High-Fidelity Simulations for Turbulent Flows

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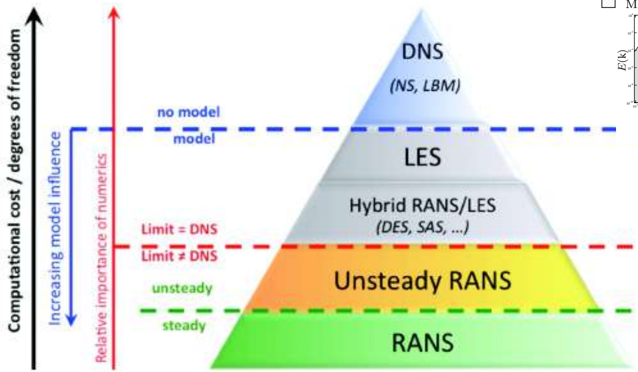
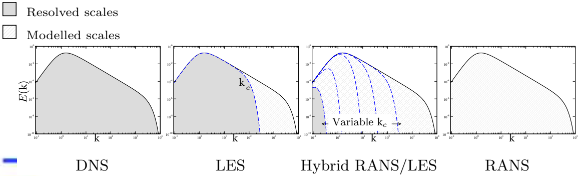
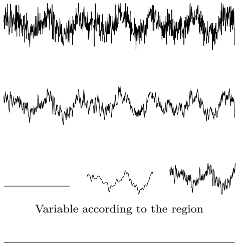
Part III

Large Eddy Simulation for compressible flows

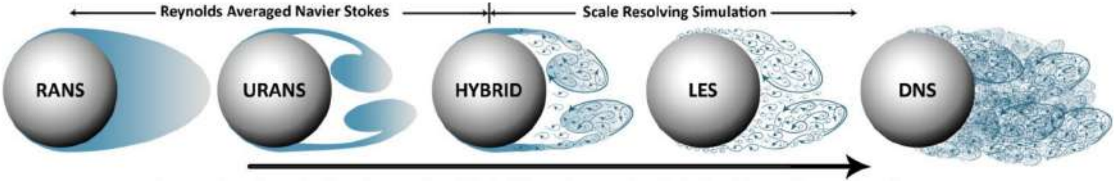
Hierarchy of CFD methods







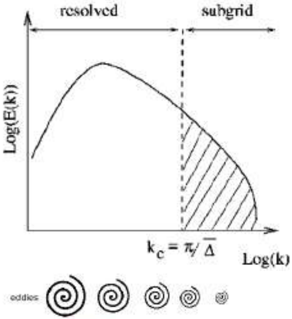
DNS	Avail.: 2080
LES	Avail.: 2070 Cost wall region $\simeq$ DNS Avail. : 2045 with wall functions
Hybrid	Avail.: 2000 Rapid development
RANS	Avail.: 1985 Industrial standard



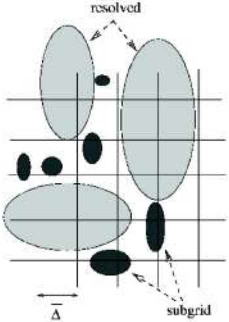
Large-Eddy Simulations (LES)

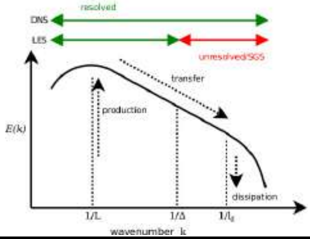
Large scales resolved and small scales modeled, κ_c defining the scales separation

Fourier space



Physical space





Comparison LES - DNS (Moin and Mahesh, 1998)

$$N_{\mathrm{LES}} \sim \frac{0.4 N_{\mathrm{DNS}}}{Re_\tau^{1/4}}$$

Re_H	Re_τ	N_{DNS}	N_{LES}
12 300	360	6.7×10^6	6.1×10^5
30 800	800	4.0×10^7	3.0×10^6
61 600	1450	1.5×10^8	1.0×10^7
230 000	4650	2.1×10^9	1.0×10^8

- LES, no walls: $N = Re^{0.5}$
- LES, walls: $N = Re^{2.4}$
- $N_{\mathrm{RANS}} = 10^4$..

✔ Reduced computational effort (5-10 % w.r.t. DNS)

✔ Modeling part restricted to small (universal) scales

✔ Allows unsteady 3D computations of coherent structures

✘ Still expensive, notably for wall-bounded flows

✘ Extension to complex geometries not trivial

✘ Filter interacts with discretization: **need for accurate schemes!**

Filtering operation: the homogeneous case

Spatial filtering: we want to compute only the "large-scale" contribution of a flow variable ϕ. How to accomplish separation?

- Apply a low-pass filter removing all the contributions smaller than a given length, corresponding to the filter width $\overline{\Delta}$
- Leonard (1974) proposes to model the filter as the application of a convolution filter to the exact solution: a filtered quantity is

$$\overline{\phi}(\vec{x},t) = \int G(\overline{\Delta}, \vec{x}-\vec{x}')\phi(\vec{x}',t)\,\mathrm{d}\vec{x}' = G_{\overline{\Delta}} \star \phi(\vec{x},t)$$

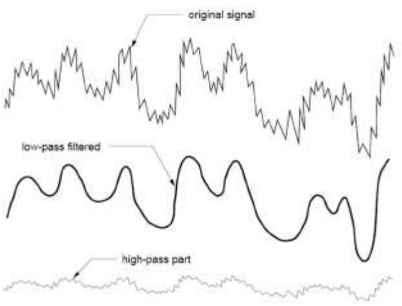
$G(\overline{\Delta}, \vec{x}-\vec{x}')$: filter kernel; $\overline{\Delta}$: cut-off length

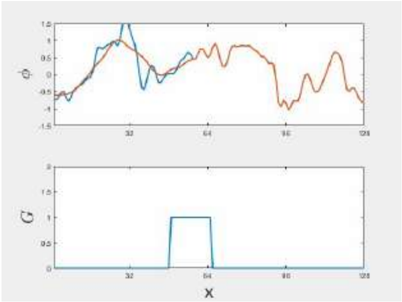
- Any quantity can be written as $\phi = \overline{\phi} + \phi'$, with $\overline{\phi} = G_{\overline{\Delta}} \star \phi$ and ϕ' the subgrid-scale (sgs) part
- The $(\vec{x}-\vec{x}')$ dependency indicates that G is homogeneous
- A convolution is a multiplication in the spectral space:

$$\widehat{\overline{\phi}}(\vec{k}) = \widehat{G}(\vec{k})\widehat{\phi}(\vec{k})$$

$\widehat{G}(\vec{k})$ being the transfer function associated to the kernel $G(\overline{\Delta}, \vec{x})$

Recall: a convolution is an integral expressing the amount of overlap of one function G as it is shifted over ϕ





LES Filter

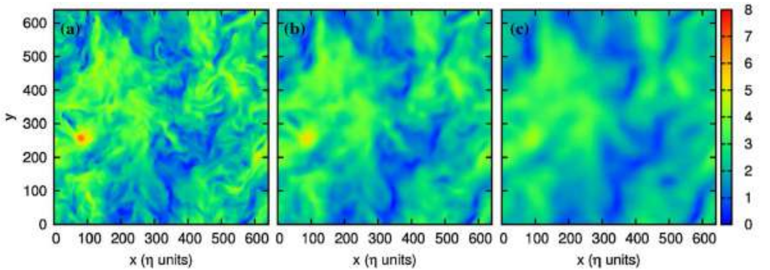


Fig. 1 Effect of filtering of the flow structures (identified by means of a 2D slice of the fluid vorticity) in HIT. **a** DNS, no filter applied, **b** LES with filter width $\Delta = 5\eta_K$, **c** LES with filter width $\Delta = 10\eta_K$, where η_K is the Kolmogorov length scale. The

✔ $\overline{\Delta}$ prescribed: control over required resolution and computational effort

✘ ..But closure problems and info reduction..

Spatio-temporal filtering: to compute the spatial and temporal large-scale contribution, one has similarly:

$$\overline{\phi}(\vec{x}, t) = \iint G(\overline{\Delta}, \overline{\theta}, \vec{x} - \vec{x}', t - t')\phi(\vec{x}', t')\,\mathrm{d}x'\,\mathrm{d}t'$$

where $G(\overline{\Delta}, \overline{\theta}, |x - x'|, t - t')$ is the filter kernel, $\overline{\Delta}$ the cut-off length, and $\overline{\theta}$ the cut-off time

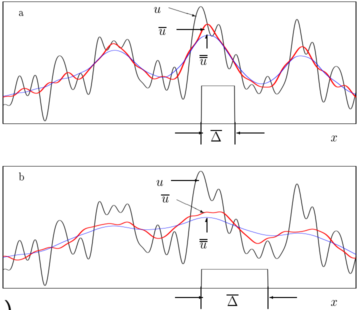
- Almost all authors consider *spatial filtering only*. Eulerian time-domain filtering has been recently revisited by Pruett et al. (2003, 2006), who considered causal filters of the form $G = G(\overline{\theta}, t - t')$.

Filter fundamental properties

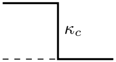
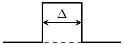
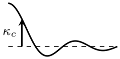
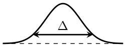
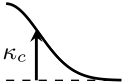
1. Linearity: $\overline{u+v} = \overline{u} + \overline{v}$ (automatically satisfied for convolution flt.)
2. Preservation of the constant: $\overline{a} = a \Leftrightarrow \int G(\overline{\Delta}, |\vec{x} - \vec{x}'|)\, \mathrm{d}\vec{x}' = 1, \forall \vec{x}$
3. Commutation with derivatives: $\left[\dfrac{\partial}{\partial x}, G\star\right] = 0 \implies \overline{\dfrac{\partial \phi}{\partial x_i}} = \dfrac{\partial \overline{\phi}}{\partial x_i}$

- These hold for Reynolds and Favre average operators
- A filter operation is not *a priori* idempotent, i.e.

$$\overline{\overline{\phi}} \neq \overline{\phi} \quad \text{and} \quad \overline{\phi'} = \overline{\phi} - \overline{\overline{\phi}} \neq 0$$



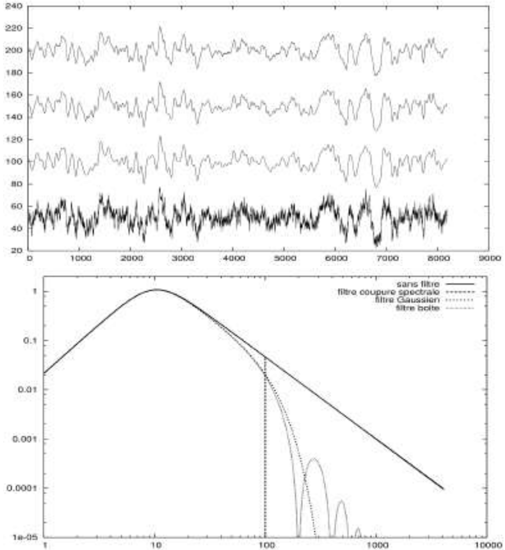
Commonly used filter kernels ($\Delta = \pi/\kappa_c$)

Filter	Kernel in physical space, G		Kernel in spectral space, $\widehat{G}$	
Spectral cutoff	$\dfrac{\sin(\pi x/\Delta)}{\pi x/\Delta}$		$\begin{cases} 1 & \text{if} \quad \lvert\kappa\rvert < \kappa_c = \pi/\Delta \\ 0 & \text{otherwise} \end{cases}$	
"Tophat" (box)	$\begin{cases} \dfrac{1}{\Delta} & \text{if} \quad \lvert x\rvert < \dfrac{\Delta}{2} \\ 0 & \text{otherwise} \end{cases}$		$\dfrac{\sin(\frac{\pi}{2}\frac{\kappa}{\kappa_c})}{\frac{\pi}{2}\frac{\kappa}{\kappa_c}}$	
Gaussian	$\sqrt{\dfrac{6}{\pi\Delta^2}} \exp\left(-\dfrac{6x^2}{\Delta^2}\right)$		$\exp\left(-\dfrac{\pi^2}{24}\dfrac{\kappa^2}{\kappa_c^2}\right)$	

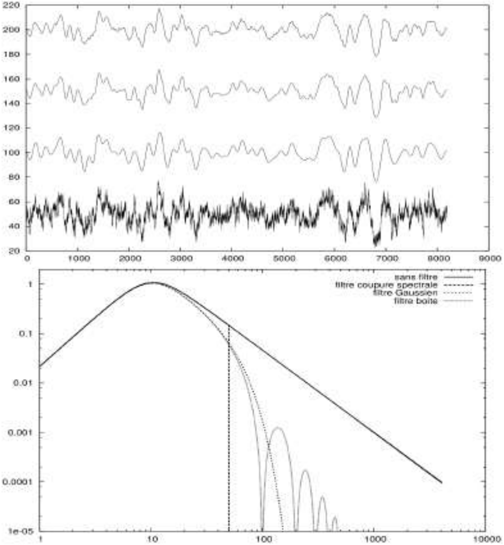
Commonly used filter kernels

From top to bottom: box, gaussian, spectral, no filter

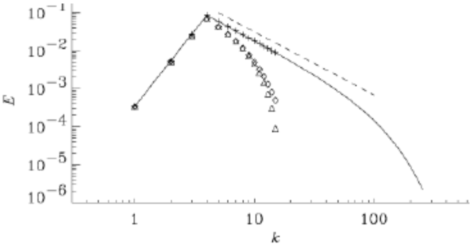
Cutoff at $\kappa_c = 100$



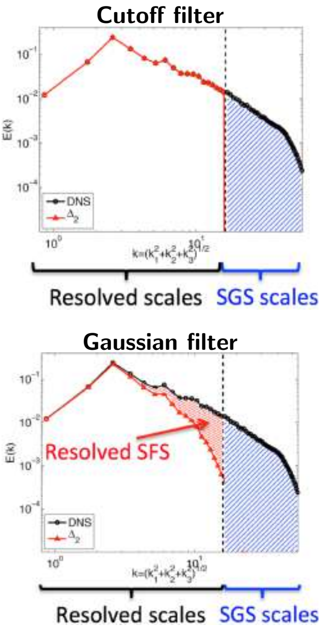
Cutoff at $\kappa_c = 50$



Commonly used filters kernels (2)



- (———) Not filtered
- (— — —) $k^{-5/3}$ slope
- (+) Spectral cut-off filter
- (◊) Gaussian filter
- (△) "Tophat" or box filter



Filter	**Physical space**	**Spectral space**
Spectral	non-local	local
Box	local	non-local
Gaussian	semilocal	semilocal

- Filter support not compact $\implies$ attenuation of energy at $\kappa < \kappa_c$
  - Scales affected are called resolved SGSs

Remarks on the filter width

Choice of the filter width

- $\overline{\Delta}$ should be sufficiently:
  - small to explicitly compute the large scales
  - large to reduce the cost w.r.t. DNS
- The corresponding grid size should be:
  - larger than $\overline{\Delta}$ (smaller is useless!)
  - sufficiently fine to solve the eddies of size $\overline{\Delta}$
- Classical choices are:
  - For homogeneous Cartesian meshes:

$$\overline{\Delta} = \Delta_x \, (= \Delta_y = \Delta_z)$$

    In this case: implicit filtering ($\neq$ ILES!)
  - For anisotropic Cartesian meshes:

$$(\Delta_x \Delta_y \Delta_z)^{1/3} \qquad \max(\Delta_x, \Delta_y, \Delta_z)$$
$$[(\Delta_x^2 + \Delta_y^2 + \Delta_z^2)/3]^{1/2}$$

  - For unstructured meshes:

$$\overline{\Delta} = (\text{Volume})^{1/3}$$

Remark: grid convergence difficult in LES (but sensitivity of statistics can be studied)

Limitation of homogeneous filters

- Modification of the support at the boundaries
  - *Problem similar to using high-order FD schemes*
- The spatial variation of the solution may vary sensibly
  - Using a variable $\overline{\Delta}$ for the filter is desirable
  - *Problem similar to using a variable grid size*

An inhomogeneous filter may be written as:

$$\overline{\phi}(\vec{x}, t) = \int G_{\overline{\Delta}}(\vec{x}, \vec{x}')\phi(\vec{x}', t)\, \mathrm{d}\vec{x}'$$

- Commutation with derivative does not hold anymore
  $\implies$ Introduction of a commutation error

$$\varepsilon_r = \overline{\frac{\partial \phi}{\partial x_i}} - \frac{\partial \overline{\phi}}{\partial x_i}$$

  - Difficult *a priori* quantification; generally, limiting the spatial variation of $\overline{\Delta}$ bounds its amount
  - In practice, ε_r often neglected with the hypothesis (unjustified?) that modeling errors are much larger..

Generic conservation law

- Let us consider the following conservation law

$$\frac{\partial \varphi}{\partial t} + \nabla \cdot \mathcal{F}(\varphi,\varphi) = 0$$

  where the nonlinear flux function $\mathcal{F}$ exhibits a quadratic behavior with respect to u.
- Applying the convolution filter, one obtains

$$\overline{\frac{\partial \varphi}{\partial t}} + \overline{\nabla \cdot \mathcal{F}(\varphi,\varphi)} = 0$$

- Applying the commutation property, this relation simplifies as

$$\frac{\partial \overline{\varphi}}{\partial t} + \nabla \cdot \overline{\mathcal{F}(\varphi,\varphi)} = 0$$

- The last step consists in rewriting the filtered nonlinear flux $\overline{\mathcal{F}(\varphi,\varphi)}$ as a function of the new filtered unknown $\overline{\varphi}$ with $\varphi = \overline{\varphi} + \varphi'$:

$$\frac{\partial \overline{\varphi}}{\partial t} + \nabla \cdot \overline{\mathcal{F}(\overline{\varphi},\overline{\varphi})} = -\nabla \cdot \left(\overline{\mathcal{F}(\overline{\varphi},\varphi')} + \overline{\mathcal{F}(\varphi',\overline{\varphi})} + \overline{\mathcal{F}(\varphi',\varphi')} \right)$$

  - The r.h.s. terms cannot be exactly computed because they explicitly depend on φ'
  - They will be *approximated* through a subgrid model, which is a function of $\overline{\varphi}$

Filtered Incompressible Navier-Stokes equations

Incompressible case:

$$\frac{\partial \overline{u}_i}{\partial x_i} = 0$$

$$\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial \overline{(u_i u_j)}}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_j} + \nu \frac{\partial^2 \overline{u}_i}{\partial x_j^2}$$

$$\frac{\partial \overline{u}_i}{\partial x_i} = 0$$

$$\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial \overline{u}_i \overline{u}_j}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_j} + \nu \frac{\partial^2 \overline{u}_i}{\partial x_j^2} - \frac{\partial \tau_{ij}^{sgs}}{\partial x_j}$$

Leonard's decomposition:

$$\begin{aligned} \tau_{ij}^{sgs} &= \overline{u_i u_j} - \overline{u}_i \overline{u}_j \\ &= \overline{(\overline{u}_i + u_i')(\overline{u}_j + u_j')} - \overline{u}_i \overline{u}_j \\ &= \underbrace{\overline{u_i' u_j'}}_{\tau_{ij}^R} + \underbrace{\overline{\overline{u}_i \overline{u}_j} - \overline{u}_i \overline{u}_j}_{\tau_{ij}^L} + \underbrace{\overline{\overline{u}_i u_j'} + \overline{u_i' \overline{u}_j}}_{\tau_{ij}^C} \end{aligned}$$

- These equations govern the evolution of large scales, which represent most of the energy (80-90%)
- The effect of small scales appears through the **subgrid-scale (SGS) stress tensor, to be modeled**:

$$\overline{u_i u_j} = \overline{u}_i \overline{u}_j + \tau_{ij}^{sgs} \implies \boxed{\tau_{ij}^{sgs} = \overline{u_i u_j} - \overline{u}_i \overline{u}_j}$$

- **Reynolds stress tensor** $\tau_{ij}^R = R_{ij}$
  - interactions between the filtered small scales
  - "true" sgs stress tensor, *unknown*
- **Leonard's tensor** $\tau_{ij}^L = L_{ij}$
  - Interaction between the large resolved scales
  - Can be explicitly computed if filter is explicit
- **Cross term tensor** $\tau_{ij}^C = C_{ij}$
  - Interaction between large and small scales
  - Difficult to model; most of the time *neglected or implicit*

- These terms represent different physical processes and should be modelled separately; in practice, τ_{ij}^{sgs} is usually modelled as a whole
- For an idempotent filter: $L_{ij} = C_{ij} = 0 \implies \tau_{ij} = R_{ij}$

Energy transfer between resolved and subgrid scales

Filtering the kinetic energy: $\overline{E}_k = \frac{1}{2}\overline{u_i u_i} = \underbrace{\frac{1}{2}\overline{u}_i\overline{u}_i}_{\text{Resolved energy}} + \underbrace{\frac{1}{2}\left(\overline{u_i u_i} - \overline{u}_i\overline{u}_i\right)}_{\text{Subgrid-scale energy}} = \widehat{E}_k + k_{sgs}$

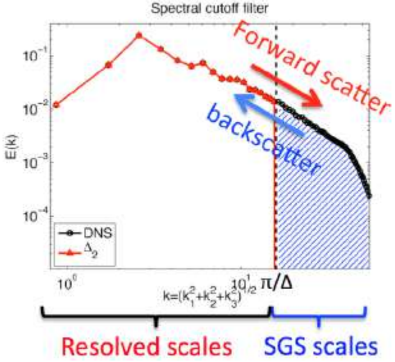
Transport equation for $\widehat{E}$

$$\overline{u}_i \times \mathcal{N}(\overline{u}_i)$$

$$\overline{u}_i\frac{\partial \overline{u}_i}{\partial t} + \overline{u}_i\frac{\partial \overline{u}_i\overline{u}_j}{\partial x_j} = -\overline{u}_i\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i} + \overline{u}_i\nu\frac{\partial^2 \overline{u}_i}{\partial x_j^2} - \overline{u}_i\frac{\partial \tau_{ij}^{sgs}}{\partial x_j}$$

$$\frac{\partial \widehat{E}}{\partial t} + \overline{u}_j\frac{\partial \widehat{E}}{\partial x_j} = -\underbrace{\frac{1}{\rho}\frac{\partial \overline{u}_i\overline{p}}{\partial x_i}}_{\text{Pressure transport}} - \underbrace{\frac{\partial \overline{u}_i\tau_{ij}^{sgs}}{\partial x_j}}_{\tau_{ij}^{sgs}\text{ transport}} - \underbrace{2\nu\frac{\partial \overline{u}_i\overline{S}_{ij}}{\partial x_j}}_{\text{viscous stress transport}} - \underbrace{\overbrace{2\nu\overline{S}_{ij}\overline{S}_{ij}}^{\widehat{\varepsilon}}}_{\text{viscous stress dissipation}} + \underbrace{\overbrace{\tau_{ij}^{sgs}\overline{S}_{ij}}^{-\varepsilon_{sgs}}}_{\text{sgs stress dissipation}}$$

$$\frac{\partial \langle E\rangle}{\partial t} + \langle u_i\rangle\frac{\partial \langle E\rangle}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \langle u_i\rangle\langle p\rangle}{\partial x_j} - \mathcal{P} - 2\nu\frac{\partial \langle u_i\rangle\langle S_{ij}\rangle}{\partial x_j} - \langle\varepsilon\rangle \qquad \text{(RANS)}$$



- ε_{sgs} is a sink for $\widehat{E}$ on average
  $\varepsilon_{sgs} > 0$: Forward scatter
  $\varepsilon_{sgs} < 0$: Backward scatter
- Similitude between averaged/filtered fields
- For high-*Re* flows, $\langle\widehat{E}\rangle = \langle E\rangle$ and the dominant sinks are

$$\left.\begin{array}{ll}\langle\varepsilon_{sgs}\rangle & \text{for } \langle\widehat{E}\rangle \\ \langle\varepsilon\rangle & \text{for } \langle E\rangle\end{array}\right\} \implies \text{one has} \quad \langle\varepsilon_{sgs}\rangle = \langle\varepsilon\rangle$$

- Recall from K41: $\langle\varepsilon\rangle \propto$ energy transfer

$\implies$ Calculating the correct $\langle\varepsilon_{sgs}\rangle$ is a necessary condition for a SGS model!

Favre-Filtered Navier–Stokes equations

- Filtering the continuity eq., we end up with $\overline{\rho u_i}$
  - To avoid this, Favre filtering:

$$\widetilde{\varphi} = \frac{\overline{\rho\varphi}}{\overline{\rho}} \qquad \Longrightarrow \qquad \overline{\rho\varphi} \equiv \overline{\rho}\widetilde{\varphi}$$

  - Favre does not commute with derivatives

The set of filtered NS eqs results from 3 choices:

1. **The filter** (usually same as in incompressible)
2. **The original set of unfiltered vars/eqs**
   - For momentum u_i, ρu_i..
   - For energy E, H, e, T, p, s..
3. **The set of filtered variables**
   - $(\overline{p},\ \widetilde{T},\ \widetilde{E})$, $(\overline{p},\ \widetilde{T},\ \check{E})$, $(\check{p},\ \check{T},\ \widetilde{E})$..

$$\overline{\rho}\widetilde{E} = \frac{\overline{p}}{\gamma-1} + \frac{1}{2}\rho\widetilde{u}_k\widetilde{u}_k + \frac{\tau_{kk}^{\text{sgs}}}{2}$$
$$= \overline{\rho}c_v\widetilde{T} + \frac{1}{2}\rho\widetilde{u}_k\widetilde{u}_k + \frac{\tau_{kk}^{\text{sgs}}}{2}$$

Examples

1. Set: π, θ, $\widetilde{E}$ (Lesieur and Comte, 2001)

$$\pi \stackrel{\text{def}}{=} \overline{p} + \frac{1}{3}\tau_{kk}, \qquad \theta = \widetilde{T} + \frac{\tau_{kk}}{2\overline{\rho}c_v}$$

$$\pi = \overline{\rho}R\theta - \frac{3\gamma-5}{6}\tau_{kk}, \qquad \overline{\rho}\widetilde{E} = \overline{\rho}c_v\theta + \frac{1}{2}\rho\widetilde{u}_i\widetilde{u}_i$$

   - π and θ macro-pressure and temperature
   - τ_{kk} requires *a priori* modeling (recast as a $f(M_{\text{sgs}})$)

2. Set: $\check{p}$, θ, $\widetilde{E}$ ("System 2" of Vreman et al., 1995)

$$\check{p} = \overline{p} + \frac{\gamma-1}{2}\tau_{kk}, \qquad \theta = \widetilde{T} + \frac{\tau_{kk}}{2\overline{\rho}c_v}$$

$$\check{p} = \overline{\rho}R\theta, \qquad \widetilde{E} = \frac{\check{p}}{\gamma-1} + \frac{1}{2}\rho\widetilde{u}_i\widetilde{u}_i$$

3. Set: $\overline{p}$, $\widetilde{T}$, $\widehat{E}$ ("System 1" of Vreman et al., 1995)

$$\overline{\rho}\widehat{E} = \frac{\overline{p}}{\gamma-1} + \frac{1}{2}\overline{\rho}\widetilde{u}_i\widetilde{u}_i$$

   - "Computable" part of the total energy
   - No change in thermodynamic variables

Favre-filtered Navier–Stokes equations

With "System 2" of Vreman (1995) formulation:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial(\overline{\rho}\widetilde{u}_i)}{\partial x_i} = 0$$

$$\frac{\partial \overline{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u}_i\widetilde{u}_j}{\partial x_j} + \frac{\partial \overline{p}}{\partial x_i} - \frac{\partial \widehat{\sigma}_{ij}}{\partial x_j} = -\frac{\partial \tau_{ij}^{sgs}}{\partial x_j} + \frac{\partial(\overline{\sigma}_{ij} - \widehat{\sigma}_{ij})}{\partial x_j}$$

$$\frac{\partial \widehat{E}}{\partial t} + \frac{\partial(\widehat{E} + \overline{p})\widetilde{u}_j}{\partial x_j} - \frac{\partial \widehat{\sigma}_{ij}\widetilde{u}_i}{\partial x_j} + \frac{\partial \widetilde{q}_j}{\partial x_j} = -B_1 - B_2 - B_3 + B_4 + B_5 + B_6 - B_7$$

p-u SGS term $\quad B_1 = \dfrac{1}{\gamma - 1}\dfrac{\partial(\overline{pu_j} - \overline{p}\widetilde{u}_j)}{\partial x_j}$

compressibility effects $\quad B_2 = \overline{p\dfrac{\partial u_k}{\partial x_k}} - \overline{p}\dfrac{\partial \widetilde{u}_k}{\partial x_k}$

kinetic energy transfer from resolved to SGS $\quad -B_3 + B_4 = -\dfrac{\partial(\tau_{kj}\widetilde{u}_k)}{\partial x_j} + \tau_{kj}\dfrac{\partial \widetilde{u}_k}{\partial x_j}$

viscous dissipation of SGS kinetic energy $\quad B_5 = \overline{\sigma_{kj}\dfrac{\partial u_k}{\partial x_j}} - \overline{\sigma}_{kj}\dfrac{\partial \widetilde{u}_k}{\partial x_j}$

SGS viscous stress $\quad B_6 = \dfrac{\partial(\overline{\sigma}_{ij}\widetilde{u}_i - \widehat{\sigma}_{ij}\widetilde{u}_i)}{\partial x_j}$

SGS heat flux $\quad B_7 = \dfrac{\partial(\overline{q}_j - \widetilde{q}_j)}{\partial x_j}$

- $\tau_{ij}^{sgs} = \overline{\rho}(\widetilde{u_i u_j} - \widetilde{u}_i\widetilde{u}_j)$
- Computable viscous stresses:

$$\widehat{\sigma}_{ij} = 2\mu(\widetilde{T})\left(\widetilde{S}_{ij} - \frac{1}{3}\widetilde{S}_{kk}\delta_{ij}\right)$$

- Computable heat flux

$$\widehat{q}_j = -\lambda\widetilde{T}\frac{\partial \widetilde{T}}{\partial x_j}$$

- $\overline{\sigma}_{ij} - \widehat{\sigma}_{ij}$ usually neglected
- Relative significance of these subgrid terms from DNS of mixing layers
  - B_1, B_2, B_3 most important terms
  - B_4 and B_5 have a weak influence
  - B_6 and B_7 (arising from T-dependency of μ and λ) generally neglected

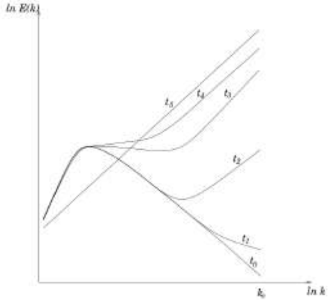
Role of SGS model

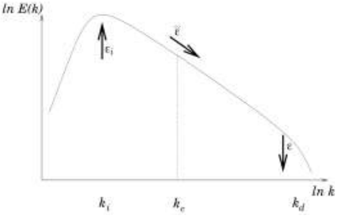
Hypothesis 1: neglect the role of subgrid scales $\Longrightarrow \tau_{ij}^{\text{sgs}} = 0$

- Underestimation of ε, mainly caused by the small scales
- If no numerical errors, energy accumulation at κ_c (end in white noise)
  - The sgs model must ensure the subgrid dissipation ε_{sgs}

Hypothesis 2: consider a steady, equilibrium configuration

- ε conditioned by large scales, $\varepsilon_i \sim \dfrac{u_i^3}{\ell_i}$, s.t. $\varepsilon = \varepsilon_i$
  - The sgs model must ensure $\varepsilon_{\text{sgs}} = \varepsilon$ to maintain equilibrium





Constraints for SGS models

- **Physical standpoint:**
  - Should be consistent, *i.e.* be zero when the flow is resolved
  - Should have the same effects on resolved scales as the true sgs scales
- **Numerical standpoint:**
  - The extra cost must be acceptable
  - Should be local in space and time
  - Should be numerically robust (no numerical instabilities)

Subgrid modelling: general strategies

Explicit modelling: new terms in the governing equations

Structural approach: $\tau_{ij}^{\text{sgs}} = \mathcal{F}_{ij}(\overline{u}_i)$

Model the sgs tensor, *i.e.* make the *best approximation* of the terms starting by $\overline{u}_i$

Hypotheses:

1. Universal form of the small scales (independence from the resolved motion)
2. Strong and simple scale correlation for the sgs structure to be deduced from the resolved field

Functional approach: $\dfrac{\partial \tau_{ij}^{\text{sgs}}}{\partial x_j} = \mathcal{F}_{ij}(\overline{u}_i)$

Model the sgs force/dissipation, *i.e.* model the *action* of the terms on $\overline{u}_i$ (not the terms themselves!)

Hypotheses:

1. The sgs action is essentially energetic: the energy transfer balance is sufficient to describe their action
2. Transfer analogous to molecular diff. mechanisms
3. Total separation between sgs and resolved scales
4. Flow in spectral equilibrium, no energy accumul.

✘ New terms to compute, can be expensive

✔ $\overline{\Delta}$ can be independent of grid size, potential for grid-independence

Implicit modelling: no new terms in the equations

- Some numerical schemes introduce diffusive errors, equivalent to a numerical viscosity ν_{num}
- Find a scheme whose dissipation properties act as an explicit sgs model even if $\tau_{ij}^{\text{sgs}} = 0$

✔ Cheap

✔ Robust

✘ Variable grids makes this "implicit filter" approximate

✘ Grid refinement changes ν_{num}, grid-dependent solution

Traditional closures for subgrid scales

- **Eddy viscosity models**: *turbulent sgs diffusion is analogous to molecular diffusion*
  - Smagorinsky (Smagorinsky, 1963)
  - Wall-Adapting Local Eddy-Viscosity (WALE) (Nicoud and Ducros, 1999)
  - Two-point closure models: Spectral eddy-viscosity (Kraichnan, 1976; Chollet and Lesieur, 1981)
    Structure function (Lesieur and Metais, 1996)
- **Dynamic Models**: *model constants become variables. Procedure applicable to any base model*
  - Dynamic Smagorinsky (Germano et al., 1991)
  - Dynamic k_{sgs}-equation (Chai and Mahesh, 2012)
- **Scale similarity models**: *the most active sgs are those close to the cutoff wavenumber*
  (Bardina et al., 1980; Liu et al., 1994; Meneveau and Katz, 2000)
- **Mixed scale models**: *combinations of two previous ones*
  (Zang et al., 1992; Horiuti, 1997; Lenormand et al., 2000)

Other approaches in LES

- **Defiltering or deconvolution:** *effects of filter/numerical errors reconstructed from the resolved field*
  - Inverse operator, assuming that high-order polynomials can be retrieved by the inversion (Geurts, 1997)
  - Exact expansion w.r.t. the derivatives of the resolved velocity (Carati et al., 2001); the first term of the expansion corresponds to the diffusivity model proposed by Leonard (1973) and Clark et al. (1979);
  - Approximate Deconvolution Model (ADM) (Stolz and Adams, 1999) based on the iterative deconvolution procedure of van Cittert, $G^{-1} \approx Q_N = \Sigma_{\nu=0}^{\infty}(I-G)^{\nu}$.

- **Regularization procedures:** *mimicking dissipative mechanisms by using appropriate numerical procedures*
  - Explicit filtering (Bogey and Bailly, 2006; Visbal and Rizzetta, 2002)
  - For the ADM model, the regularization is obtained by subtracting a relaxation term (Stolz et al., 2001);
  - The regularization can arise directly from the numerical discretization scheme as in the MILES (Monotonically-Integrated LES) method (Boris et al., 1992)
  - A dynamic SM model can provide a sufficient regularization level (Gullbrand and Chow, 2003)

- **Multiscale approaches:** *scale decomposition constructed considering that sgs effects are limited to the interactions with resolved scales with a size at least twice*
  - Subgrid-scale tensor estimation model (Domaradzki and Saiki, 1997);
  - *Ab initio* scale separation in the wavenumber space (Hughes et al., 2001);
  - Turbulent hyperviscosity models (Winckelmans et al., 1996; Vreman, 2003).

Eddy viscosity models

Boussinesq's hypothesis: $\tau_{ij}^{sgs,D} = \tau_{ij}^{sgs} - \frac{\delta_{ij}}{3}\tau_{kk}^{sgs} = 2\nu_{sgs}\left(\widetilde{S}_{ij} - \frac{\delta_{ij}}{3}\widetilde{S}_{kk}\right) = 2\nu_{sgs}\widetilde{S}_{ij}^{D}$

- Only deviatoric part taken into account (isotropic part added to macro-pressure $\pi = \overline{p} + \overline{\rho}\tau_{kk}/3$);
- sgs supposed homogeneous and isotropic: a simple algebraic model is sufficient to model them

$$\nu_{sgs} \sim \ell_{sgs} u_{sgs} = \ell_{sgs}^2 / t_{sgs}$$

- Most active SGS motions near the cut-off $\Longrightarrow$ the natural ℓ_{sgs} is $\approx \overline{\Delta}$
- Natural u_{sgs} chosen as $u_{sgs}^2 = k_{sgs}$, or $t_{sgs} = \frac{1}{|\overline{S}_{ij}|}$ with $|\overline{S}_{ij}| = \sqrt{2\overline{S}_{ij}\overline{S}_{ij}}$

One-equation models
(Schumann, 1975)

Prescribe ℓ_{sgs}, u_{sgs} predicted by the flow:

$$u_{sgs} \propto \sqrt{k_{sgs}}, \quad \nu_t = C_1 \ell_{sgs}\sqrt{k_{sgs}}, \quad \tau_{ij}^{sgs} = -2C_1\ell_{sgs}\sqrt{k_{sgs}}\overline{S}_{ij}$$

- A transport equation for k_{sgs} is needed:

$$\frac{\partial k_{sgs}}{\partial t} + \frac{\partial \overline{u}_j k_{sgs}}{\partial x_j} = 2\nu_t \overline{S}_{ij}\overline{S}_{ij} - \varepsilon + \frac{\partial}{\partial x_j}\left(2\nu_t \frac{\partial k_{sgs}}{\partial x_j}\right)$$

- $C_1 = 0.1$, $\ell_{sgs} = \overline{\Delta}$, $\varepsilon = C\frac{k_{sgs}^{3/2}}{\ell_{sgs}}$ with C damp. func.

Two-equations models
(Deardorff, 1973)

Predict both ℓ_{sgs} and u_{sgs} by the flow

- Example: model the evolution of τ_{ij}^{sgs}
- Approach similar to RSM RANS closures
- ✘ Larger computational cost
- ✘ Same limitation of other EVM approaches

Smagorinsky model

Precursor of subgrid modeling (Smagorinsky, 1963), based on local equilibrium. ε_{sgs} is

$$\varepsilon_{\text{sgs}} = -\tau_{ij}^{\text{sgs}}\overline{S}_{ij} = 2\nu_{\text{sgs}}\overline{S}_{ij}\overline{S}_{ij} = \nu_{\text{sgs}}|\overline{S}_{ij}|^2 \qquad \text{with} \qquad \nu_{\text{sgs}} \propto u_{\text{sgs}}\overline{\Delta}$$

For equilibrium, $\varepsilon_{\text{sgs}} = \varepsilon \approx \dfrac{u_i^3}{\ell_i} \implies$ one can assume $\varepsilon_{\text{sgs}} = \nu_{\text{sgs}}|\overline{S}_{ij}|^2 \propto u_{\text{sgs}}\overline{\Delta}|\overline{S}_{ij}|^2 \propto \dfrac{u_{\text{sgs}}^3}{\overline{\Delta}} \implies u_{\text{sgs}} \propto \overline{\Delta}|\overline{S}_{ij}|$

Resulting in $\boxed{\nu_{\text{sgs}} = C_s u_{\text{sgs}}\overline{\Delta} = (C_s\overline{\Delta})^2|\overline{S}_{ij}|}$ and $\boxed{\varepsilon_{\text{sgs}} = (C_s\overline{\Delta})^2|\overline{S}_{ij}||\overline{S}_{ij}|^2 = (C_s\overline{\Delta})^2|\overline{S}_{ij}|^3}$

with C_s the Smagorinsky constant. **How to estimate its value?**

Assume a Kolmogorov spectrum: $E(k) = C_k\varepsilon^{2/3}\kappa^{-5/3}$ with $\kappa \in [0, \kappa_c]$ and $C_k \approx 1.41$. Then

$$\langle|\overline{S}_{ij}|^2\rangle = \langle 2\overline{S}_{ij}\overline{S}_{ij}\rangle \simeq 2\int_0^{\kappa_c}\kappa^2 E(\kappa)\,\mathrm{d}\kappa = 2C_k\varepsilon^{2/3}\int_0^{\kappa_c}\kappa^{1/3}\,\mathrm{d}\kappa = \frac{3}{2}C_k\varepsilon^{2/3}\left(\frac{\pi}{\overline{\Delta}}\right)^{4/3}$$

Rearranging for ε and imposing $\varepsilon_{\text{sgs}} = \varepsilon$, we get:

$$\left(\frac{2}{3C_k}\right)^{3/2}\langle|\overline{S}_{ij}|^2\rangle^{3/2}\left(\frac{\pi}{\overline{\Delta}}\right)^2 = \langle(C_s\overline{\Delta})^2|\overline{S}_{ij}|^3\rangle \qquad \implies \qquad C_s \simeq \frac{1}{\pi}\left(\frac{2}{3C_k}\right)^{3/4} \simeq 0.18$$

- ✔ Robust, easy to implement
- ✘ Generally too dissipative
- ✘ C_s not an "universal value" (0.1 often used)
- ✘ Need for van Driest damping function at the wall
- ✘ Not for transition ($\nu_{\text{sgs}} \geq 0$ even for laminar flows)
- ✘ Does not allow backscatter

Compressible extension of SM

- The isotropic part of the subgrid tensor τ_{kk} must also be modeled. The model of Yoshizawa (1986) reads:

$$k_{sgs} = C_I \overline{\Delta}^2 |\overline{S}_{ij}|^2$$

  - To estimate C_I, the same procedure of SM is used. k_{sgs} is

$$\langle k_{sgs} \rangle = \int_{\kappa_c}^{\infty} E(\kappa)\,\mathrm{d}\kappa = C_k \varepsilon^{2/3} \int_{\kappa_c}^{\infty} \kappa^{-5/3} = \frac{3}{2} C_k \varepsilon^{2/3} \left(\frac{\pi}{\overline{\Delta}}\right)^{-2/3} = \langle |\overline{S}_{ij}|^2 \rangle \left(\frac{\pi}{\overline{\Delta}}\right)^{-2}$$

  Therefore, $$\langle |\overline{S}_{ij}|^2 \rangle \left(\frac{\pi}{\overline{\Delta}}\right)^{-2} = C_I \overline{\Delta}^2 |\overline{S}_{ij}|^2 \implies C_I = \frac{1}{\pi^2} \approx 0.1.$$

  - Erlebacher et al. (1992) estimate $C_I = 0.066$ from DNS of CHIT

- For the energy equation, taking Vreman's formulation:

$$B_1 + B_2 = -\frac{\partial}{\partial x_j}\left(\frac{c_p \overline{\rho} \nu_{sgs}}{Pr_t} \frac{\partial \widetilde{T}}{\partial x_j}\right) = \frac{\partial Q_j}{\partial x_j}$$

  where the value of Pr_t can be chosen around 0.6.

- SM prescribes both u_{sgs} and ℓ_{sgs}
- Subsequent models improve adaptation of ν_{sgs} to local flow properties

Wall-Adapting Local Eddy-Viscosity (WALE) model

Nicoud and Ducros (1999) criticize SM model:

1. Both S_{ij} and Ω_{ij} contribute to global dissipation
2. Near-wall damping functions are *ad hoc* models

The general form of EV models is

$$\nu_{\text{sgs}} = C_m \overline{\Delta}^2 \overline{\text{OP}(\vec{x}, t)}$$

- $\text{OP}(\vec{x}, t)$ should have the following properties:
  - invariant to rotation or translation
  - easily assessed on any computational grid
  - function of both S_{ij} and Ω_{ij}
  - goes naturally to 0 at the wall

$\Longrightarrow$ **Wall-Adapting Local Eddy-Viscosity (WALE) model**

- They consider the traceless symmetric part of the square of the velocity gradient tensor

$$G^D_{ij} = \frac{1}{2}(\overline{A}^2_{ij} + \overline{A}^2_{ji}) - \frac{\delta_{ij}}{3}\overline{A}^2_{kk} \quad \text{with} \quad A_{ij} = \frac{\partial \overline{u}_i}{\partial x_j} \quad \text{and} \quad \overline{A}^2_{ij} = \overline{A}_{ik}\overline{A}_{kj}$$

- WALE model is given as

$$\nu_{\text{sgs}} = (C_w \Delta)^2 \frac{\left(G^D_{ij} G^D_{ij}\right)^{3/2}}{\left(\overline{S}_{ij}\overline{S}_{ij}\right)^{5/2} + \left(G^D_{ij} G^D_{ij}\right)^{5/4}} \qquad \text{with} \qquad C_w \approx \sqrt{10.6}\, C_s$$

✔ Deficiencies of SM model alleviated

✔ Correct behavior of ν_{sgs} (≈ 0 in wall-bounded laminar flows)

✔ Local formulation

Structure function models

- Based on spectral model of Kraichnan (1976), *i.e.* $\nu_{\text{sgs}} = \frac{2}{3} C_k^{-3/2} \sqrt{\frac{E(\kappa_c)}{\kappa_c}}$ with $\kappa_c = \frac{\pi}{\Delta}$
- **Idea** of Lesieur and Metais (1996): go beyond SM keeping this same scaling in physical space
  - To evaluate $E_{\vec{x}}$ in the physical space, use the second-order structure function of velocity flucts.:

$$F_2(\overline{\Delta}, t) = \langle \| \vec{u}(\vec{x} + \vec{r}, t) - \vec{u}(\vec{x}, t) \|^2 \rangle_{\|\vec{r}\| = \overline{\Delta}}$$

For HIT, Batchelor relation:

$$F_2(\overline{\Delta}, t) = 4 \int_0^{\kappa_c} E(\kappa, t) \left[1 - \frac{\sin(\kappa \overline{\Delta})}{\kappa \overline{\Delta}} \right] \mathrm{d}\kappa$$

Starting from the Kolmogorov spectrum, the SF model is:

$$\nu_{\text{sgs}} = C_F \overline{\Delta} \sqrt{\overline{F}_2(\vec{x}, \overline{\Delta}, t)}$$

$$\text{with} \quad C_F \simeq 0.105 C_k^{-3/2}$$

- In practice, $\overline{F}_2$ is computed locally by averaging neighboring points; i.e., for a Cartesian 2D grid:

$$\begin{aligned} F_2(\overline{\Delta}, t) = \frac{1}{4} \{ & [\vec{u}(x + \overline{\Delta}, y, t) - \vec{u}(x, y, t)]^2 + \\ & [\vec{u}(x - \overline{\Delta}, y, t) - \vec{u}(x, y, t)]^2 + \\ & [\vec{u}(x, y + \overline{\Delta}, t) - \vec{u}(x, y, t)]^2 + \\ & [\vec{u}(x, y - \overline{\Delta}, t) - \vec{u}(x, y, t)]^2 \} \end{aligned}$$

- Formulation very close to SM:

$$\lim_{\overline{\Delta} \to 0} \nu_t(\vec{x}, t) \approx 0.777 \left(C_s \overline{\Delta} \right)^2 \sqrt{2 \overline{S}_{ij} \overline{S}_{ij} + \overline{\omega}_{ij} \overline{\omega}_{ij}}$$

✔ Less dissipative in almost laminar zones or in presence of a weak vorticity

✘ More dissipative where strong velocity gradients are present

Dynamic models

- The models presented include coeffs to be prescribed either based on
  - Theory with specific assumptions (isotropy)
  - Calibration with experimental data
  - A posteriori results

Can we avoid this?

- Germano et al. (1991) developed a procedure to evaluate **dynamically** unknown model constants
  - It can be applied to any model coeff (C_s, Pr_{sgs}, C_I,..)
  - The constants become space- and time-dependent (Moin et al., 1991)
  - and depend as little as possible on the level of filtered velocity on which the prediction is based

Dynamic Models - Germano's identity

- The base idea is to apply a second filter (test filter) (Lilly, 1992) at a larger scale (say $2\overline{\Delta}$):
  - Add a separation between largest scales ($\overline{\overline{u}}_i$ or $\widehat{\overline{u}}_i$) and smallest resolved scales ($\overline{u}_i - \overline{\overline{u}}_i$ or $\overline{u}_i - \widehat{\overline{u}}_i$);
  - Smallest resolved scales act similar to the largest ones to be modelled, $\overline{u_i'}$ (indirectly relying on scale-similarity structural concepts)

$$\widehat{\frac{\partial \overline{u}_i}{\partial t}} + \widehat{\frac{\partial (\overline{u}_i \overline{u}_j)}{\partial x_j}} = -\widehat{\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i}} + \nu \widehat{\frac{\partial^2 \overline{u}_i}{\partial x_j^2}} - \widehat{\frac{\partial \tau_{ij}^{sgs}}{\partial x_j}}$$

$$\frac{\partial \widehat{\overline{u}}_i}{\partial t} + \underbrace{\frac{\partial \widehat{(\overline{u}_i \overline{u}_j)}}{\partial x_j}}_{I} = -\frac{1}{\rho}\frac{\partial \widehat{\overline{p}}}{\partial x_i} + \nu \frac{\partial^2 \widehat{\overline{u}}_i}{\partial x_j^2} - \underbrace{\frac{\partial \widehat{\tau}_{ij}^{sgs}}{\partial x_j}}_{II}$$

$$\frac{\partial \widehat{\overline{u}}_i}{\partial t} + \frac{\partial (\widehat{\overline{u}}_i \widehat{\overline{u}}_j)}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \widehat{\overline{p}}}{\partial x_i} + \nu \frac{\partial^2 \widehat{\overline{u}}_i}{\partial x_j^2} - \frac{\partial \left[(\widehat{\overline{u_i u_j}}) - (\widehat{\overline{u}}_i \widehat{\overline{u}}_j) \right]}{\partial x_j}$$

$$\frac{\partial \widehat{\overline{u}}_i}{\partial t} + \frac{\partial (\widehat{\overline{u}}_i \widehat{\overline{u}}_j)}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \widehat{\overline{p}}}{\partial x_i} + \nu \frac{\partial^2 \widehat{\overline{u}}_i}{\partial x_j^2} - \frac{\partial \mathcal{T}_{ij}}{\partial x_j}$$

Term I: $\dfrac{\partial \widehat{(\overline{u}_i \overline{u}_j)}}{\partial x_j} = \dfrac{\partial (\widehat{\overline{u}}_i \widehat{\overline{u}}_j)}{\partial x_j} + \dfrac{\partial \left[\widehat{(\overline{u}_i \overline{u}_j)} - (\widehat{\overline{u}}_i \widehat{\overline{u}}_j) \right]}{\partial x_j}$

Term II: $\dfrac{\partial \widehat{\tau}_{ij}^{sgs}}{\partial x_j} = \dfrac{\partial (\widehat{\overline{u_i u_j}})}{\partial x_j} - \dfrac{\partial \widehat{(\overline{u}_i \overline{u}_j)}}{\partial x_j}$

- Red terms cancel out
- Noting that
  1. $\tau_{ij}^{sgs} = \overline{u_i u_j} - \overline{u}_i \overline{u}_j$
  2. $\mathcal{T}_{ij} = \widehat{\overline{u_i u_j}} - \widehat{\overline{u}}_i \widehat{\overline{u}}_j$
  3. $\mathcal{L}_{ij} = \widehat{\overline{u}_i \overline{u}_j} - \widehat{\overline{u}}_i \widehat{\overline{u}}_j$

  Combining 1, 2 and 3 one has **Germano's identity**

$$\boxed{\mathcal{L}_{ij} = \mathcal{T}_{ij} - \widehat{\tau}_{ij}^{sgs}}$$

Dynamic Models - Germano's identity

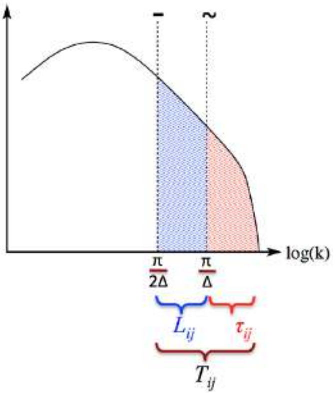
$$\frac{\partial \widehat{\overline{u}}_i}{\partial t} + \frac{\partial (\widehat{\overline{u}}_i \widehat{\overline{u}}_j)}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \widehat{\overline{p}}}{\partial x_i} + \nu \frac{\partial^2 \widehat{\overline{u}}_i}{\partial x_j^2} - \frac{\partial \mathcal{T}_{ij}}{\partial x_j} \quad \text{with} \quad \mathcal{T}_{ij} = \widehat{\overline{u_i u_j}} - \widehat{\overline{u}}_i \widehat{\overline{u}}_j \quad \text{and} \quad \mathcal{L}_{ij} = \mathcal{T}_{ij} - \widehat{\tau}_{ij}$$

- The identity is exact and is known explicitly
- Can be used to dynamically compute coeffs for any base SGS model
- The classical (and most famous) is the **Dynamic Smagorinsky Model**

The two subgrid tensors τ_{ij} and $\mathcal{T}_{ij}$ respectively associated with $\overline{\Delta}$ and $\widehat{\Delta}$ are modeled by a Smagorinsky-like expression:

$$\tau_{ij}^D = \tau_{ij} - \frac{\delta_{ij}}{3}\tau_{kk} = -2(C_s\overline{\Delta})^2|\overline{S}_{ij}|\overline{S}_{ij} = -2C_d\mathcal{B}_{ij}$$

$$\mathcal{T}_{ij}^D = \mathcal{T}_{ij} - \frac{\delta_{ij}}{3}\mathcal{T}_{kk} = -2(C_s\widehat{\Delta})^2|\widehat{\overline{S}}_{ij}|\widehat{\overline{S}}_{ij} = -2C_d\mathcal{A}_{ij}$$



Thus, from Germano's identity:

$$\mathcal{L}_{ij}^D = \mathcal{L}_{ij} - \frac{\delta_{ij}}{3}\mathcal{L}_{kk} \equiv \mathcal{T}_{ij}^D - \widehat{\tau}_{ij}^D \overset{\text{SM}}{=} -2(C_d\mathcal{A}_{ij} - \widehat{C_d\mathcal{B}_{ij}}) = -2C_d\mathcal{M}_{ij} \qquad \text{where} \quad \mathcal{M}_{ij} = \mathcal{A}_{ij} - \widehat{\mathcal{B}}_{ij}$$

- It is assumed $\widehat{C_d\mathcal{B}_{ij}} \approx C_d\widehat{\mathcal{B}}_{ij}$, corresponding to the commutation error (small if C_d variations are on scales much larger than $\hat{\Delta}$)

Dynamic Models - DSM

$$\mathcal{L}_{ij}^D = \mathcal{L}_{ij} - \frac{\delta_{ij}}{3}\mathcal{L}_{kk} \equiv \mathcal{T}_{ij}^D - \widehat{\tau}_{ij}^D \overset{\text{SM}}{=} -2C_d\mathcal{M}_{ij} \qquad \mathcal{M}_{ij} = \mathcal{A}_{ij} - \widehat{\mathcal{B}}_{ij}$$

- Overdetermined system! (6 equations, 1 relation for C_d)
- Germano et al. (1991) proposes to obtain C_d by contracting with $\overline{S}_{ij}$ ensemble averaging:

$$C_d = -\frac{1}{2}\frac{\mathcal{L}_{ij}^D\overline{S}_{ij}}{\mathcal{M}_{ij}\overline{S}_{ij}}$$

✘ Denominator can be zero numerically, unstable formulation

- Lilly (1992) proposes to write an expression for the error associated to SM model in Germano's identity:

$$E_{ij} = \mathcal{L}_{ij}^D - 2C_d\mathcal{M}_{ij}$$

and use a least-square approach to compute the "best fit" by minimizing the squared error w.r.t. C_d:

$$E_{ij}^2 = (\mathcal{L}_{ij}^D - 2C_d\mathcal{M}_{ij})^2 = (\mathcal{L}_{ij}^D)^2 - 4C_d\mathcal{L}_{ij}^D\mathcal{M}_{ij} + 4C_d^2\mathcal{M}_{ij}^2 \implies \frac{\partial E_{ij}^2}{\partial C_d} = -4\mathcal{L}_{ij}^D\mathcal{M}_{ij} + 8C_d\mathcal{M}_{ij}^2$$

$$\frac{\partial E_{ij}^2}{\partial C_d} = 0 \quad \implies \quad -4\mathcal{L}_{ij}^D\mathcal{M}_{ij} + 8C_d\mathcal{M}_{ij}^2 = 0 \quad \implies \quad C_d = \frac{1}{2}\frac{\mathcal{L}_{ij}^D\mathcal{M}_{ij}}{\mathcal{M}_{ij}^2}$$

Remarks:

- Model very popular, although the implementation is tricky and expensive
- $\widehat{\Delta} = 2\overline{\Delta}$ generally chosen for test filter width
- $\nu + \nu_{\text{sgs}} \leq 0$ must be avoided by using a local average or an average in homogeneous directions
- Often less dissipative than SM (smaller ν_{sgs}) but remains generally overdissipative at high Re

Dynamic Models

- **Problem 1:** C_d varies strongly in space and contains a significant fraction of negative values
  $\Longrightarrow$ the assumption $\widehat{C_d \mathcal{B}_{ij}} \approx C_d \widehat{\mathcal{B}_{ij}}$ not completely justified! **Possible solutions**:
  - Perform ensemble averages on homogeneous directions, *i.e.* $C_d = \frac{1}{2} \frac{\langle \mathcal{L}_{ij}^D \mathcal{M}_{ij} \rangle}{\langle \mathcal{M}_{ij}^2 \rangle}$ or $C_d = \frac{1}{2} \left\langle \frac{\mathcal{L}_{ij}^D \mathcal{M}_{ij}}{\mathcal{M}_{ij}^2} \right\rangle$
  - Clipping the value by imposing $\nu_{\text{sgs}} + \nu \geq 0$ and $C_d \leq C_{\max}$
  - Minimization of C_d along particle trajectories (Meneveau et al., 1996)

- **Problem 2**: We assumed that C_s^2 applies at both scales, *i.e.* $C_s^2(\Delta) = C_s^2(2\Delta)$
  Good if $\Delta/2\Delta$ in the inertial range, bad for anisotropic flows (e.g. near the BL wall). **Possible solution**:
  - Generalized dynamic model (Porté-Agel et al., 2000), with C_s^2 function of scale, *e.g.* $\frac{C_s^2(2\Delta)}{C_s^2(\Delta)} = \frac{C_s^2(4\Delta)}{C_s^2(2\Delta)}$

✔ Compatible with near-wall regions

✔ fully-resolved regions where ν_{sgs} should nullify

✔ good for LTT transition

✘ C_d values (under/overdiffusion to be avoided)!

Another dynamic approach is the **Dynamic k_{sgs}-equation**

- "Static" evaluation from Yoshizawa and Horiuti (1985)
- "Dynamic" compressible from Chai and Mahesh (2012)
  Solve the transport equation for k_{sgs} and use $\sqrt{k_{\text{sgs}}}$ as ℓ_{sgs}
- All coeffs C_s, Pr_t, C_f, $C_{\varepsilon s}$, $C_{\varepsilon c}$ are determined dynamically

$$\tau_{ij} - \frac{2}{3}\overline{\rho} k_{\text{sgs}} \delta_{ij} = -2 C_s \Delta \overline{\rho} \sqrt{k_{\text{sgs}}} \widetilde{S}_{ij}^D$$

$$q_j = -\frac{\mu_t}{Pr_t} \frac{\partial \widetilde{T}}{\partial x_j} = -\frac{C_s \Delta \overline{\rho} \sqrt{k_{\text{sgs}}}}{Pr_t} \frac{\partial \widetilde{T}}{\partial x_j}$$

Multiscale Smagorinsky model (MSM)

First introduced by Hughes et al. (1998) as the *Variational Multiscale Model* (VMM)

- Resolved part separated in small and large resolved scales: $\overline{u} = u^{>} + u^{<}$
  - $u^{>}$ represents the large scales, $u^{<}$ the medium scales
- The decomposition is introduced in the subgrid scale, which keeps the same expression:

$$\tau_{ij}^{\text{sgs},D} = \tau_{ij}^{\text{sgs}} - \frac{\delta_{ij}}{3}\tau_{kk}^{\text{sgs}} = 2\nu_{\text{sgs}}\left(\overline{S}_{ij}^{<} - \frac{1}{3}\delta_{ij}\overline{S}_{kk}^{<}\right)$$

- The sgs viscosity can also be expressed from the larger, smaller scales, or both:
  - "Large-small" version (*MSM - ls*): $\nu_{\text{sgs}} = C_s^2\overline{\Delta}^2|\overline{S}_{ij}|$
  - "Small-small" version (*MSM - ss*): $\nu_{\text{sgs}} = C_s^2\overline{\Delta}^2|\overline{S}_{ij}^{<}|$
  - C_s is constant, but can also be computed dynamically (replacing SM by DSM)
    $\Longrightarrow$ *Multiscale Dynamic Smagorinsky Model*, MDSM
- A test filter is required to operate the scale separation
- The precise location of the scale separation has a weak influence (Holmen et al., 2004; Jeanmart and Winckelmans, 2007)

Scale Similarity model or Bardina's model

This structural model does not rely on the eddy viscosity concept, but on a scale similarity hypothesis (Bardina et al., 1980). The subgrid scale tensor is modelled as

$$\boxed{\tau_{ij} = \overline{\overline{u}_i \overline{u}_j} - \overline{\overline{u}}_i \overline{\overline{u}}_j} \qquad \text{or} \qquad \boxed{\tau_{ij} = \widetilde{\overline{u}_i \overline{u}_j} - \widetilde{\overline{u}}_i \widetilde{\overline{u}}_j}$$

Base idea:

- Add a separation between the largest scales ($\overline{\overline{u}}_i$ or $\widetilde{\overline{u}}_i$) and the smallest resolved scales ($\overline{u}_i - \overline{\overline{u}}_i$ or $\overline{u}_i - \widetilde{\overline{u}}_i$);
- The smallest resolved scales act similar to the largest ones to be modelled, $\overline{u'_i}$.
  - A double filtering operations shows indeed that $\overline{u}_i - \overline{\overline{u}}_i = \overline{\overline{u}_i + u'_i} - \overline{\overline{u}}_i = \overline{\overline{u}}_i + \overline{u'_i} - \overline{\overline{u}}_i = \overline{u'_i}$

Recalling Leonard's decomposition, Bardina's model reads:

$$\begin{cases} \tau_{ij}^R = \overline{u'_i u'_j} \approx \overline{u'_i}\,\overline{u'_j} = \left(\overline{u}_i - \overline{\overline{u}}_i\right) \cdot \left(\overline{u}_j - \overline{\overline{u}}_j\right) \\ \tau_{ij}^C = \overline{u'_i \overline{u}_j} + \overline{\overline{u}_i u'_j} \approx \overline{u'_i}\,\overline{\overline{u}}_j + \overline{\overline{u}}_i\,\overline{u'_j} = \left(\overline{u}_i - \overline{\overline{u}}_i\right) \overline{\overline{u}}_j + \overline{\overline{u}}_i \left(\overline{u}_j - \overline{\overline{u}}_j\right) \\ \tau_{ij}^L = \overline{\overline{u}_i \overline{u}_j} - \overline{u}_i \overline{u}_j \end{cases} \implies \quad \tau_{ij} = \tau_{ij}^L + \tau_{ij}^C + \tau_{ij}^R = \overline{\overline{u}_i \overline{u}_j} - \overline{\overline{u}}_i \overline{\overline{u}}_j$$

- ✔ Mathematical approximation $\implies$ no physical modeling required
- ✔ Correlates better with measurements than Boussinesq hypothesis (Liu et al., 1994)
- ✔ Much better estimation for the exact τ_{ij}^{sgs} w.r.t. EVM
- ✘ Not enough dissipative $\rightarrow$ computation not stable if applied alone
- ✘ Cannot be applied if the filter is idempotent
- ✘ Computational cost

Mixed-Scales models

- Scale-similarity models underestimate dissipation and are unstable
  - Mix with more robust and dissipative EVM! $\Longrightarrow$ **Mixed-scale models**

For instance (Zang et al., 1992): Bardina's similarity model + the SM or DSM

$$\tau_{ij} - \frac{\delta_{ij}}{3}\tau_{kk}^{sgs} = \frac{1}{2}\left(2\nu_{sgs}\overline{S}_{ij} + L_{ij} - \frac{1}{3}L_{kk}\right)$$

with

$$\nu_{sgs} = (C_s\overline{\Delta})^2\sqrt{2\overline{S}_{ij}\overline{S}_{ij}} \qquad \text{and} \qquad L_{ij} = \overline{\overline{u}_i\overline{u}_j} - \overline{\overline{u}}_i\overline{\overline{u}}_j$$

Remarks:

- One of the best models when ν_{sgs} evaluated dynamically
- the value of C_s is reduced around 0.01

Evaluation and testing of SGS models

How should models be **validated** and **compared** to each other? Pope (2004) gives 5 criteria:

1. The **accuracy** of the model
   - Ability to reproduce DNS, experimental, or theoretical statistical features of a given test flow
   - Ability to converge to these values with increasing resolution $\Longrightarrow$ grid convergence
2. The **cost and ease of use** of the model
   - One model may give better results at lower grid resolution (larger $\overline{\Delta}$) but with excessive costs
3. The **completeness** of the model
   - Handle different flows with different BCs, ICs, forcings..
4. Level of description in the SGS model
5. The range and applicability of the model

A posteriori testing

Run "full" simulations with SGS model and compare results to DNS, experiments or theory

✔ Complete test of the model ("dynamic" feedback)

✘ Model quality influenced by numerics

A priori testing

Use DNS or high-resolution experimental data to test SGS models "offline"

✔ Test quality of the model

✘ Does not include dynamic feedback and numerics..

Numerical errors in LES

- Numerical schemes introduce dissipation and dispersion errors altering the numerical representation of a given solution mode
  - The smallest structures are the worst represented, albeit they play a crucial role (turbulence, aeroacoustics, discontinuities, ..)
  - In LES, the smallest resolved scales carry much more energy w.r.t. DNS

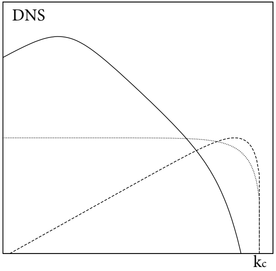
  ↪ Paramount importance of discretization!

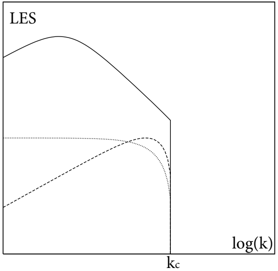
Example: consider $\overline{u}$ and its spatial derivative $\dfrac{\partial \overline{u}}{\partial x}$. In Fourier space:

$$\widehat{\frac{\partial \overline{u}}{\partial x}}(\kappa) \begin{array}{ll} = i\kappa \widehat{G}(\kappa)\widehat{u}(\kappa) & \text{Exact derivative} \\ = i\kappa_{\text{eff}}\widehat{G}(\kappa)\widehat{u}(\kappa) = i\kappa \widehat{G}_{\text{eff}}(\kappa)\widehat{u}(\kappa) & \text{Numerical evaluation} \end{array}$$

- κ replaced by a modified wavenumber $\kappa_{\text{eff}}(\kappa)$, depending on the num. scheme
  - κ_{eff} increases and then drops to 0 at $\kappa = \kappa_c$, determined by the grid
  - For DNS, κ_c pushed to the right; For LES, κ_c in the inertial range
  - The value $\kappa - \kappa_{\text{eff}}$ depends on accuracy of FD formula
  - Computing a derivative with $\kappa_{\text{eff}} \neq \kappa$ amounts to replacing $\widehat{G}(\kappa)$ by $\widehat{G}_{\text{eff}}(\kappa) = \dfrac{\kappa_{\text{eff}}}{\kappa}\widehat{G}(\kappa) \implies$ additional filtering

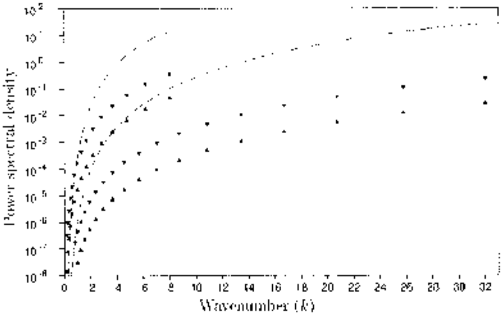
Numerical errors can be **one order of magnitude greater than the subgrid modelling** if the spatial discretization is second-order accurate



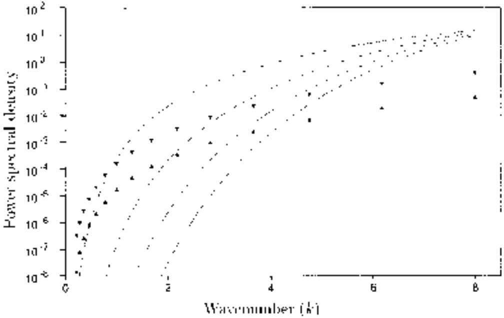


Solid: $\overline{u}$, Dashed: κ_{eff}
Dotted: $\kappa_{\text{eff}}/\kappa$

Numerical errors in LES (2)



FD errors of a 2nd-order scheme (———) w.r.t. lower (▲) and upper (▼) bounds of the sgs force for $k_m = 8$ and 32 (Ghosal, 1996; Kravchenko and Moin, 1997)



FD errors (———) w.r.t. lower (▲) and upper (▼) bounds of the sgs force for $k_m = 8$. The schemes shown are 2nd, 4th, 6th and 8th-order (highest to lowest curve) central diff.

- Error for low-order schemes cannot be sufficiently reduced by refining the grid (the sgs contribution also decreasing as the grid is refined), unless $\overline{\Delta}$ is considerably larger than the grid size
- Higher-order schemes lead to reduced levels of error
- Even with an 8th-order scheme, the subgrid contribution is dominated by numerical errors in about half of the wavenumber range!

The effective filter

The **effective filter** observed in practical LES originates from very different sources:

1. *The theoretical filter*
   - Applied to the exact solution of the NS
   - Its characteristic length is $\overline{\Delta}$
2. *The grid filter*
   - No scale smaller than Δ_x can be captured
   - The cut-off wavenumber is $\kappa_c = \pi/\Delta_x$ on uniform grids (Nyquist criterion)
3. *The numerical filter*
   - The numerical error is not uniformly distributed over the resolved wavenumbers
   - The dynamics of the highest frequencies resolved on the grid is only poorly captured
4. *The subgrid model filter*
   - It is the only term with info related to the convolution filter (e.g., through $\overline{\Delta}$)
   - The fact that SGS models are not exact modifies the original filter

Grid resolution requirements

- Visc. dissip. in $0.1 \leq \kappa\eta \leq 1$, i.e. $6 \leq L/\eta \leq 60$
  - Resulting criterion for DNS is $\Delta x \sim \eta$

DNS (Moin and Mahesh, 1998)

Flow	Resolution ($\eta = [\nu^3/\varepsilon]^{1/4}$)		
	$\Delta x/\eta$	$\Delta y/\eta$	$\Delta z/\eta$
Boundary layer	14	0.33	5
Homogeneous shear	8	4	4
Isotropic turbulence	4.5	4.5	4.5

- Wall-bounded flows induce drastic constraints
  - No scale separation (inertial range disappears): Impossible to apply a filter separating energ. and dissip. ranges; all scales must be resolved
  - For $Re > 10^5$, $> 90\%$ of grid points are used in $< 10\%$ of the simulation domain (near walls)

What can we do? Two strategies available:

Wall-Resolved LES (WR-LES): Solve inner layer

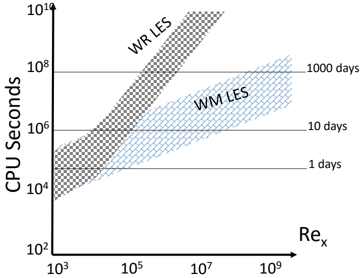
- Most SGS models not applicable near the wall (homogeneous hyp.) $\implies$ changes needed

Ex: VD damping $C_s' = C_s \left[1 - \exp\left(-\frac{y^+}{A}\right)\right]$

Boundary Layer flow

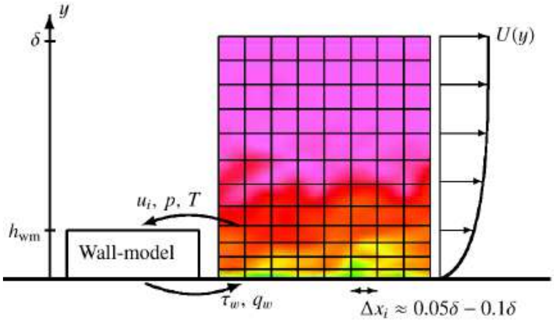
	DNS	WRLES
Δx^+	10	50 – 100
Δy^+_{min}	0.33	1
Δz^+	5	10 – 20

Wall-Modeled LES (WM-LES): Model inner layer

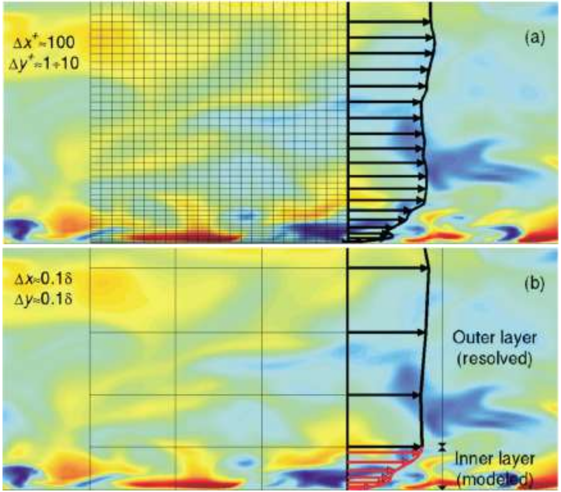


Wall-Modeled LES

- Model the inner layer and use approximate wall BCs
- **Two existing approaches**:
  1. Switch to RANS formulation
     ↪ Hybrid RANS/LES
  2. Model directly τ_w s.t. $\tau_w = f(\overline{u})$
     ↪ Wall-stress-modeled LES (WSMLES)



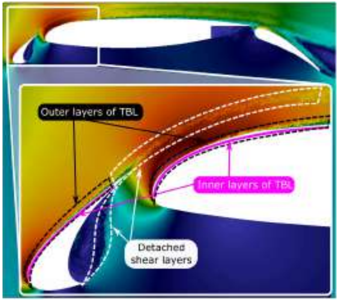
Piomelli and Balaras (2002)



Similar ideas used in RANS (wall functions), WM-LES, hybrid RANS/LES models, ...
More difficult in LES since treatment must be valid for an unsteady resolved field

Wall-stress-modeled LES

Larsson et al. (2016)



(a) Detached shear layer
(b) Outer layers of TBL
(c) Inner layers of TBL

- Hybrid RANS/LES solves (a)
- WMLES solves (a) and (b)
  - Potential for more accuracy in non-equilibrium flows

- Even a **perfect WM** would not be able to accurately predict C_f
  - It is fed underresolved info from LES $\Longrightarrow$ **Math-based approaches**
- Otherwise, **physics-based approaches**:

$$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u u_j}{\partial x_j} + \frac{\partial p}{\partial x} = \frac{\partial}{\partial y}\left[(\mu + \mu_{sgs}^{wm})\frac{\partial u}{\partial y}\right]$$

1. Equilibrium conditions: $l.h.s. = 0$, ODE obtained (solution is the usual wall law)
2. Equilibrium model can be implemented either by
   - Algebraically solving the log-law for u_τ
   - Numerically solving the ODE directly

$$\frac{\mathrm{d}}{\mathrm{d}y}\left[(\mu + \mu_{sgs}^{wm})\frac{\mathrm{d}u}{\mathrm{d}y}\right] = 0$$

$$\frac{\mathrm{d}}{\mathrm{d}y}\left[c_p\left(\frac{\mu}{Pr} + \frac{\mu_{sgs}^{wm}}{Pr_t}\right)\frac{\mathrm{d}T}{\mathrm{d}y}\right] = -\frac{\mathrm{d}}{\mathrm{d}y}\left[(\mu + \mu_{sgs}^{wm})u\frac{\mathrm{d}u}{\mathrm{d}y}\right]$$

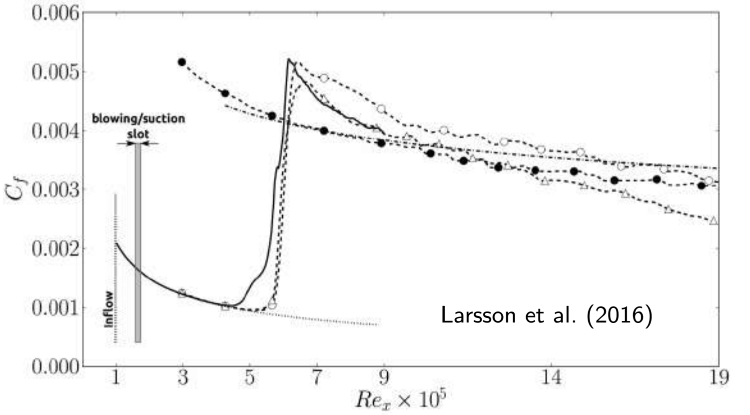
with $\mu_{sgs}^{wm} = \rho\kappa\sqrt{\frac{\tau_w}{\rho}}y\left[1 - \exp\left(-\frac{y^+}{A^+}\right)\right]^2$

3. Non-equilibrium conditions: resolve directly the full BL PDEs

✘ Classical problem is the "log-layer $\overline{u}^+$ mismatch" (also for hybrid!)

✘ Transition to turbulence

Transition problem



) Skin friction coefficient along a flat plate boundary layer undergoing transition, for WMLES with the transition-sensor (dashed line with open circles), standard WMLES without any sensor (dashed line with filled circles), and underresolved LES on the same grid but without any wall-model at all (dashed line with open triangles). The results are compared to the DNS of Sayadi *et al.* (2013) (solid line), the theoretical laminar result $c_f = 0.664 Re_x^{-1/2}$ (lower dotted line), and the semi-analytical turbulent correlation $c_f = 0.455/[\log(0.06 Re_x)]^2$ (upper dash-dotted line). Taken from Bodart & Larsson (2012).

- Wall models assume developed turbulence
- Problem partially solved with sensors

✔ WMLES alleviates the need to resolve the inner layer

✘ It is not a license to poorly resolve the outer layer

✘ The grid has a direct effect on results

- Testing different grids is fundamental
- Both grid-refinement and aspect-ratio change

Classification of WMLES approaches

Larsson et al. (2016)

Wall-modeled LES (WMLES)
inner layer ($y/\delta \lesssim 0.2$) modeled, outer layer ($y/\delta \gtrsim 0.2$) resolved

I: Hybrid LES/RANS
LES defined only for $y \geq y_{\text{int}} > 0$

(a) seamless: y_{int} set by grid and/or solution
(DES as wall-model, IDDES, ...)
(cf. Nikitin *et al.*, 2000; Shur *et al.*, 2008, ...)

(b) zonal: y_{int} set by the user
(most LES/RANS approaches)
(cf. Baurle *et al.*, 2003; Temmerman *et al.*, 2005, ...)

II: Wall-stress-models
LES extends all the way to the wall at $y = 0$

(a) math-based: based on other than physics arguments
(control-theory, filter-based, ...)
(cf. Nicoud *et al.*, 2001; Bose & Moin, 2014, ...)

(b) physics-based: generally RANS-like models
(i) no wall-parallel grid-connectivity
(algebraic, ODE, ...)
(cf. Schumann, 1975; Kawai & Larsson, 2012, ...)
(ii) with wall-parallel grid-connectivity
(PDE, momentum integral, ...)
(cf. Balaras *et al.*, 1996, ...)

2D Hill

From Park (2017)

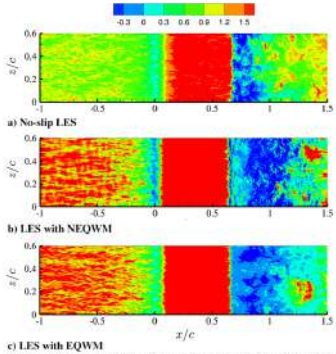
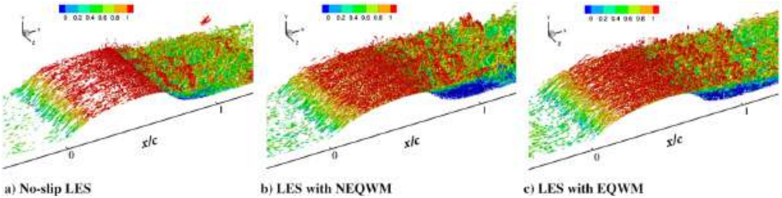


Fig. 11 Contour of the instantaneous wall-tangential shear stress (G1 grid): a) no-slip LES (no wall model), b) LES with the NEQWM, and c) LES with the EQWM.



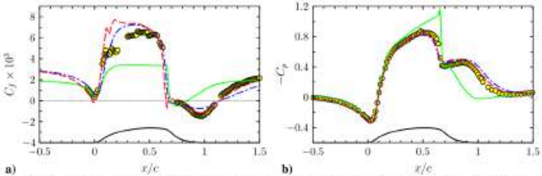
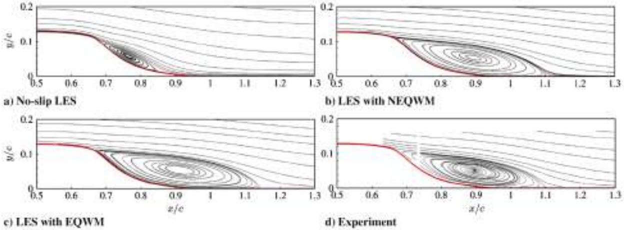
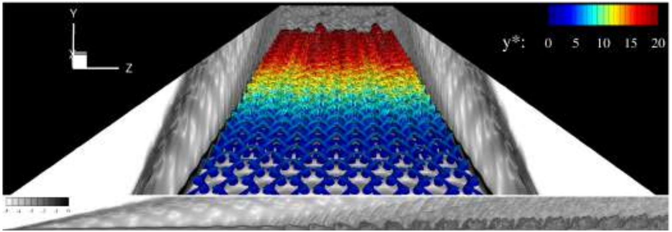


Fig. 12 a) Skin friction coefficient, and b) pressure coefficient along the bottom wall. Lines are from the present simulations run with the baseline grid (G1). Red dashed line, LES with the NEQWM; blue dashed-dotted line, LES with the EQWM; green solid line, no-slip LES; circles, experiment [42].



Boundary conditions for LES

Like all numerical techniques for PDEs,
LES requires specification of BCs and ICs



Initial conditions

Important issue for some flows (*e.g.*, HIT)

- DNS: nearly identical issues
- RANS: not so crucial

Boundary conditions

- **Wall conditions**: already described
- **Outflow**: important when unphysical numerical reflections may pollute the results (aeroacoustics, subsonic flows, reacting flows, ..)
  - Use of characteristic relations
  - Include source terms to damp specific features
- **Periodic conditions**: for homogeneous directions, domain large enough not to constrain the flow
- **Inflow conditions**: the most delicate and complex (Tabor and Baba-Ahmadi, 2010)
  - Impose a field of the same nature as the results wanted from the simulation
  - Impossible to inject real turbulence.
    The incoming velocity fluctuations should be

  ↪ stochastically varying
  ↪ ... on scales down to the filter scale
  ↪ compatible with NS eqs
  ↪ "look" like turbulence
  (intensities, length scales, spectra, ...)
  ↪ easy to implement and to adjust do new inlet conditions

Inflow conditions

- Something similar to turbulence must be imposed (spatio-temporal coherence properties)

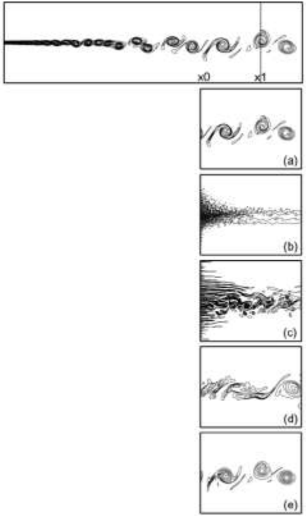


Fig. 7 Spanwise vorticity contours: top, reference simulation ($L_x = 280\delta_{\omega_0}$), a–e, truncated simulations ($L_x' = 100\delta_{\omega_0}$) using inflow conditions detailed in the text.

Simulation of a mixing layer (Druault et al., 2004)

Full simulation

(a) IC extracted from the full simulation

(b) White noise matching the energy level

(c) IC preserving temporal correlations

(d) IC preserving spatial correlations

(e) IC preserving spatio-temporal correlations

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