High-Fidelity Simulation for Turbulent Flows

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Estimation of HPC resources 1

A new turbulence model has been proposed, whose coefficients need to be calibrated by performing a DNS of homogeneous isotropic turbulence at a Reynolds number of $Re = 10^3$. In order to have access to the local High Performance Computing (HPC) resources, a proposal must be submitted with details concerning the overall cost of the simulation. The code to be used has the following characteristics:

- The sequential fraction of the code (that is, the fraction of the code that cannot be parallelized) is S = 0.002:
- The code has been previously used for the same configuration, but at Re = 200. For this Reynolds number, the total number of grid points needed to ensure DNS resolution is $N = 12 \cdot 10^6$ points and the total computational cost of the simulation is C = 1500 CPU hours.
- 1. Estimate the number of grid points for the new configuration and the total amount of CPU hours that should be demanded to carry out the simulation.

Solution: For a given configuration, we know that the number of grid points scales as $N \sim \mathrm{Re}^{9/4}$, whereas the total cost scale as $C \sim \mathrm{Re}^3$. Therefore, the number of grid points and the simulation cost for the present run will be of the order of

$$N_{\text{new}} = N_{\text{old}} \left(\frac{\text{Re}_{\text{new}}}{\text{Re}_{\text{old}}}\right)^{9/4} = 12 \cdot 10^6 \cdot \left(\frac{1000}{200}\right)^{9/4} = 448.6 \cdot 10^6 \text{ points}$$
 (1)

$$C_{\text{new}} = C_{\text{old}} \left(\frac{\text{Re}_{\text{new}}}{\text{Re}_{\text{old}}}\right)^3 = 1500 \cdot \left(\frac{1000}{200}\right)^3 = 187500 \text{ CPU hours}$$
 (2)

can estimate

2. A condition for obtaining the computational hours required is that the run should be completed in 7 days. Assuming that there is no limit in the number of cores N_{cores} that can be used and the scalability of the code is ideal, can the simulation run be completed on time?

Solution: If the scalability of the code is ideal, a code without sequential parts (S = 0) would have a speedup equal to the number of cores used. However, in this case the code has a sequential fraction of S = 0.002; the maximum achievable speedup is the "potential speedup":

 $s_{\text{pot}} = \frac{1}{S} = \frac{1}{0.002} = 500 \tag{3}$

Meaning that the code will at best run 500 times faster than the single-core code (even if one uses $N_{\text{cores}} > 500$). Therefore, the minimum time-to-solution (TTS) is equal to

$$TTS = \frac{C_{\text{new}}}{s_{\text{pot}}} = \frac{187500}{500} = 375 \text{ hours} = 15.6 \text{ days}$$
 (4)

Seven days are therefore not sufficient to complete the simulation.

3. Someone finally finds the solution to remove completely the sequential fraction of the code (thus S=0), but now unfortunately the code runs 10% slower than before. Estimate again the number of CPU hours that are needed in these new conditions and the number of cores $N_{\rm cores}$ that should be used to end the run in 7 days.

Solution: The overall computational cost will be 10% higher, hence one would need $187\,500 \cdot 1.1 = 206\,250$ CPU hours. Nevertheless, the limitation of 500 cores has been removed, and we can compute the number of cores needed to end the simulation in 7 days:

$$N_{\text{cores}} = \frac{206250}{7 \cdot 24} = 1228 \tag{5}$$

4. Determine how much time you will need to perform the simulation on a single core, assuming that the efficiency of the multi-core run is 90%

Solution: The efficiency is defined as

$$\eta = \frac{T_{\text{wc}}^{1 \text{ core}}}{T_{\text{wc}}^{N_{\text{cores}}} \cdot N_{\text{cores}}} \tag{6}$$

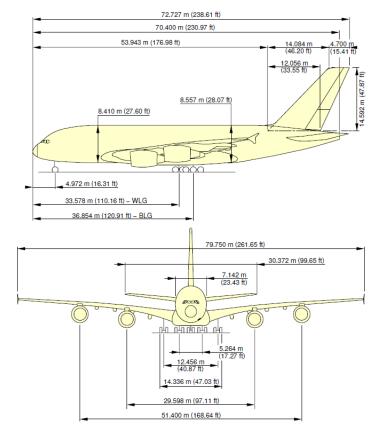
Therefore on a single-core computer one would need

$$T_{\rm wc}^{1~{\rm task}} = \eta \cdot T_{\rm wc}^{N_{\rm cores}} \cdot N_{\rm cores} = 0.9 \cdot (7 \cdot 24) \cdot 1228 = 185\,674~{\rm hours} = 21~{\rm years} \eqno(7)$$

2 Propulsion of an Airbus A380

The propulsion of an Airbus A380 is ensured by 4 engines, each one providing a thrust of $F = 300 \,\mathrm{kN}$ allowing to fly at a cruise velocity of $U = 910 \,\mathrm{km/h}$ at an altitude of $h = 10\,700 \,\mathrm{m}$, where the air properties are as follows: temperature $T = -55 \,^{\circ}\mathrm{C}$, density $\rho = 0.4 \,\mathrm{kg/m^3}$, kinematic viscosity $\nu = 4 \cdot 10^{-5} \,\mathrm{m^2 s^{-1}}$. The aim of this problem is to explore the feasibility of a Direct Numerical Simulation (DNS) of the flow around the airplane.

**ON A/C A380-800 Models A380-800F Models



1. Compute the power developed by the engines.

Solution:
$$P = n \cdot F \cdot U = 4 \cdot 300\,000 \cdot \frac{910}{3.6} \approx 3 \cdot 10^8 \,\text{W} \tag{1}$$

2. In a steady flight regime, the power developed by the engines is equal to the power dissipated by the turbulent motions of the air flow. Assuming that the air volume moved by the plane is comparable to the volume of the plane itself, compute the power per unit mass dissipated in the air flow, ε .

Solution: By neglecting the volume of the wings, the airplane may be assimilated to a cylinder, with a volume of

$$V \approx \frac{\pi}{4} \cdot (\text{diameter})^2 \cdot \text{length} = \frac{\pi}{4} \cdot 8.4^2 \cdot 70 \approx 4000 \,\text{m}^3$$
 (2)

The air volume moved by the plane is therefore

$$m_{\rm air} = \rho_{\rm air} \cdot V = 1600 \,\mathrm{kg} \tag{3}$$

and the power per unit mass dissipated in the air flow

$$\varepsilon = \frac{P}{m_{\text{air}}} = \frac{3 \cdot 10^8}{1600} \approx 1.9 \cdot 10^5 \,\text{m}^2 \text{s}^{-3}$$
 (4)

3. Derive the expression of the Kolmogorov scale η as a function of ε and ν , and compute it for the present case.

Solution: One obtains

$$\eta = \left(\frac{\nu^3}{\varepsilon}\right)^{1/4} = \left[\frac{(4 \cdot 10^{-5})^3}{1.9 \cdot 10^5}\right]^{1/4} \approx 25 \,\text{\mum}$$
(5)

4. We want to perform the DNS in a computational domain of size $6 \times$ the length, $3 \times$ the width and $3 \times$ the height of the plane. We consider a regular, cubic Cartesian mesh. Estimate the number of grid points N and the number of time steps N_t needed to run the simulation for a total time of L/U. Are these orders of magnitude achievable with modern computational resources?

Solution: The total volume of the computational domain is:

$$\begin{cases} \text{Length:} & 6 \cdot 72 \approx 432 \,\text{m} \\ \text{Width:} & 3 \cdot 80 \approx 180 \,\text{m} \implies 432 \cdot 180 \cdot 69 \approx 5.4 \cdot 10^6 \,\text{m}^3 \\ \text{Height:} & 3 \cdot 23 \approx 69 \,\text{m} \end{cases}$$
(6)

For a DNS, the grid size must be of the order of the Kolmogorov scale in each spatial dimension. Therefore the number of grid points is

$$N = \frac{L_x \cdot L_y \cdot L_z}{\eta^3} = \frac{5.4 \cdot 10^6}{(25 \cdot 10^{-6})^3} = 3.5 \cdot 10^{20}$$
 (7)

The number of time steps can be approximated as

$$N_t = \frac{\text{Total runtime}}{\text{time step}} = \frac{L_x/U}{\eta/U} = \frac{L_x}{\eta} = \frac{432}{25e - 6} \approx 17 \cdot 10^6$$
 (8)

This orders of magnitude are clearly not achievable with modern computational resources.

5. Estimate the plane surface (consider only the fuselage and the wings) and derive the stress τ_w exerted on the plane from the flow.

Solution: The total surface is

$$\begin{cases} \text{Fuselage:} & \pi \cdot 8.4 \cdot 70 \approx 1800 \,\text{m}^2 \\ \text{Wings:} & 2 \cdot 70 \cdot 12 \approx 1700 \,\text{m}^2 \end{cases} \implies S \approx 1800 + 1700 = 3500 \,\text{m}^2 \qquad (9)$$

The total stress is then

$$\tau_w = \frac{F}{S} = \frac{4 \cdot 300\,000}{3500} \approx 340\,\frac{\text{N}}{\text{m}^2}$$
(10)

6. Derive the expression of the friction velocity u_{τ} as a function of τ_w and ρ and of the viscous length δ_v , and compute u_{τ} and δ_v .

Solution: One has

$$u_{\tau} = \sqrt{\frac{\tau_w}{\rho}} \approx \sqrt{\frac{340}{0.4}} \approx 30 \,\frac{\mathrm{m}}{\mathrm{s}} \tag{11}$$

$$\delta_v = \frac{\nu}{u_\tau} = \frac{4 \cdot 10^{-5}}{30} \approx 1.4 \,\text{\mu m}$$
 (12)

7. Is the previously estimated grid sufficiently refined for resolving the viscous sublayer? What should be done if it is not the case?

Solution: The grid was estimated on a grid size of about 25 µm. Since $\delta_v \approx 1.4$ µm and we need $y^+ \approx 1$ at the walls, it will not be refined enough to capture the viscous sublayer. A wall-refined grid must be used instead, with a first cell height of about 1.4 µm.

3 LES of Homogeneous Isotropic Turbulence

A problem of homogeneous isotropic turbulence at high-Reynolds numbers is to be solved by means of Large-Eddy simulations. To this aim, we need to estimate the width of the LES filter needed in order to ensure that a given portion of the turbulent spectrum is resolved. It is assumed that, in the inertial range, the turbulent kinetic energy spectrum follows Kolmogorov's law $E(\kappa) = C\varepsilon^{2/3}\kappa^{-5/3}$, with C = 1.5 and where κ and ε denote the wavenumber and the dissipation rate of the turbulet kinetic energy k_t , respectively.

1. Define a lengthscale L as a function of k_t and ε .

Solution: From a dimensional standpoint, since $[k_t] = \frac{\text{m}^2}{\text{s}^2}$ and $[\varepsilon] = \frac{\text{m}^2}{\text{s}^3}$, one has

$$L = \frac{k_t^{3/2}}{\varepsilon} \tag{1}$$

2. For homogeneous turbulence, the filtered kinetic energy spectrum function reads

$$\overline{E}(\kappa) = \widehat{G}^2(\kappa)E(\kappa) \tag{2}$$

where $\overline{(\bullet)}$ denotes the filtering operation and $\widehat{G}(\kappa)$ the transfer function of the filter. Use equation (2) to derive a relation for computing $\langle k_{\rm sgs} \rangle$, where $k_{\rm sgs}$ denotes the subgrid-scale kinetic energy and $\langle \bullet \rangle$ a volume integration operation.

Solution: One has simply:

$$\langle k_{\rm sgs} \rangle = \langle E(\kappa) - \overline{E}(\kappa) \rangle = \langle [1 - \widehat{G}^2(\kappa)] E(\kappa) \rangle = \int_0^\infty [1 - \widehat{G}^2(\kappa)] E(\kappa) \, d\kappa$$
 (3)

3. Let's consider now an isotropic sharp spectral filter of width Δ and the related cutoff wavenumber $\kappa_c = \frac{\pi}{\Delta}$. The transfer function of such a filter reads

$$\widehat{G}(\kappa) = \begin{cases} 0 & \text{if } |\kappa| \ge \kappa_c \\ 1 & \text{if } |\kappa| < \kappa_c \end{cases} \tag{4}$$

Using the equation derived in step 2, derive a relation of the type

$$\frac{\langle k_{\text{sgs}} \rangle}{k_t} = A \cdot L^{\alpha} \cdot \kappa_c^{\beta} \tag{5}$$

where $\frac{\langle k_{\text{sgs}} \rangle}{k_t}$ denotes the ratio of the subgrid-scale kinetic energy to the total turbulent kinetic energy. Find the numerical values of the constants A, α and β .

Solution: Using equation (3) and the definition of the transfer function, the total integrated subgrid-scale kinetic energy reads

$$\langle k_{\text{sgs}} \rangle = \int_0^\infty [1 - \widehat{G}^2(\kappa)] E(\kappa) \, d\kappa = \int_0^{\kappa_c} [1 - 1^2] E(\kappa) \, d\kappa + \int_{\kappa_c}^\infty [1 - 0^2] E(\kappa) \, d\kappa \qquad (6)$$

$$= \int_{\kappa_c}^\infty E(\kappa) \, d\kappa = \int_{\kappa_c}^\infty C \varepsilon^{2/3} \kappa^{-5/3} \, d\kappa = -\frac{3}{2} C \varepsilon^{2/3} \kappa^{-2/3} \Big|_{\kappa = \kappa_c}^\infty = \frac{3}{2} C \varepsilon^{2/3} \kappa_c^{-2/3} \qquad (7)$$

Since

$$L = \frac{k_t^{3/2}}{\varepsilon} \quad \Longrightarrow \quad \varepsilon = \frac{k_t^{3/2}}{L} \tag{8}$$

Replacing in equation (6), one obtain

$$\langle k_{\text{sgs}} \rangle = \frac{3}{2} C \left(\frac{k_t^{3/2}}{L} \right)^{2/3} \kappa_c^{-2/3} = \frac{3}{2} C \frac{k_t}{L^{2/3}} \kappa_c^{-2/3}$$
 (9)

And thus

$$\frac{\langle k_{\text{sgs}} \rangle}{k_t} = \frac{3}{2} C(L\kappa_c)^{-2/3} \tag{10}$$

The values of the constants are $A = \frac{3}{2}C = 2.25$ and $\alpha = \beta = -\frac{2}{3}$.

4. What assumptions must hold for the previous result to be valid?

Solution: The Kolmogorov spectrum is valid only in the inertial range, therefore the previous result is valid if and only if the the cutoff wavenumber κ_c is contained inside the inertial range.

5. Find the value of $\frac{\Delta}{L}$ for which 75% of the turbulent kinetic energy spectrum is resolved.

Solution: If 75% of the spectrum is resolved, 25% is the portion of subgrid-scale energy. Injecting this value is equation (10), one obtains:

$$\frac{\langle k_{\text{sgs}} \rangle}{k_t} = \frac{3}{2} C(L\kappa_c)^{-2/3} = \frac{3}{2} C\left(L\frac{\pi}{\Delta}\right)^{-2/3} = 0.25$$
 (11)

And thus

$$\frac{\Delta}{L} = \pi \left(\frac{2}{3} \frac{0.25}{C}\right)^{-3/2} = 0.116\tag{12}$$

6. Repeat the same analysis of step 3 and 5 for a Gaussian filter, whose transfer function reads

$$\widehat{G}(\kappa) = \exp\left(-\frac{\kappa^2 \Delta^2}{24}\right) \tag{13}$$

In the calculations, the following result should be used:

$$I_0 \equiv \int_0^\infty (1 - e^{-x}) x^{-4/3} \, \mathrm{d}x \approx 4.062 \tag{14}$$

Solution: In this case, the value of $\langle k_{\rm sgs} \rangle$ reads

$$\langle k_{\text{sgs}} \rangle = \int_0^\infty [1 - \hat{G}^2(\kappa)] E(\kappa) \, d\kappa = \int_0^\infty \left[1 - \exp\left(-2\frac{\kappa^2 \Delta^2}{24}\right) \right] C \varepsilon^{2/3} \kappa^{-5/3} \, d\kappa \qquad (15)$$

$$= C\varepsilon^{2/3} \int_0^\infty \left[1 - \exp\left(-\frac{\kappa^2 \Delta^2}{12}\right) \right] \kappa^{-5/3} \, \mathrm{d}\kappa \tag{16}$$

One can perform a change of variables such that $x = \frac{\kappa^2 \Delta^2}{12}$, for which then

$$\kappa = \frac{\sqrt{12x}}{\Delta} \quad \text{and} \quad d\kappa = \frac{\sqrt{12}}{\Delta} \frac{dx}{2\sqrt{x}}$$
(17)

Moreover, considering that $\varepsilon^{2/3} = \frac{k_t}{L^{2/3}}$, one obtains

$$\langle k_{\rm sgs} \rangle = C \frac{k_t}{L^{2/3}} \int_0^\infty \left[1 - e^{-x} \right] \left(\frac{\sqrt{12x}}{\Delta} \right)^{-5/3} \frac{\sqrt{12}}{\Delta} \frac{\mathrm{d}x}{2\sqrt{x}}$$
 (18)

$$= C \frac{k_t}{L^{2/3}} \left(\frac{\sqrt{12}}{\Delta}\right)^{-2/3} \frac{1}{2} \int_0^\infty \left[1 - e^{-x}\right] \sqrt{x}^{-8/3} \, \mathrm{d}x \tag{19}$$

and then

$$\frac{\langle k_{\text{sgs}} \rangle}{k_t} = C \left(\frac{\Delta}{L}\right)^{2/3} 96^{-1/3} \int_0^\infty \left[1 - e^{-x}\right] x^{-4/3} \, \mathrm{d}x = C \left(\frac{\Delta}{L}\right)^{2/3} 96^{-1/3} I_0 \tag{20}$$

Since $\Delta = \frac{\pi}{\kappa_c}$, one has

$$\frac{\langle k_{\text{sgs}} \rangle}{k_t} = C \pi^{2/3} \left(\kappa_c L \right)^{-2/3} 96^{-1/3} I_0 \tag{21}$$

And thus $A = C\pi^{2/3}96^{-1/3}I_0 = 2.854$ and $\alpha = \beta = -\frac{2}{3}$.

In order to resolve 75% of the turbulent kinetic energy spectrum, one must have

$$\frac{\langle k_{\text{sgs}} \rangle}{k_t} = C \left(\frac{\Delta}{L}\right)^{2/3} 96^{-1/3} I_0 = 0.25$$
 (22)

and thus

$$\frac{\Delta}{L} = \left(\frac{0.25}{C96^{-1/3}I_0}\right)^{3/2} = \left(\frac{0.25}{1.5 \cdot 96^{-1/3} \cdot 4.062}\right)^{3/2} = 0.130\tag{23}$$

7. For a given numerical cutoff κ_c , compute the ratio of the subgrid-scale kinetic energies obtained with the two filters, $\frac{\langle k_{\rm sgs} \rangle|_{\Delta=\Delta_{\rm gauss}}}{\langle k_{\rm sgs} \rangle|_{\Delta=\Delta_{\rm spect}}}$. Which filter drains more energy? Why?

Solution: Equations (10) and (21) show that in both cases α and β are equal; therefore, the ratio $\frac{\langle k_{\text{sgs}} \rangle|_{\Delta = \Delta_{\text{gauss}}}}{\langle k_{\text{sgs}} \rangle|_{\Delta = \Delta_{\text{spect}}}}$ simply reduces to the ratio of the coefficients A:

$$\frac{\langle k_{\text{sgs}} \rangle |_{\Delta = \Delta_{\text{gauss}}}}{\langle k_{\text{sgs}} \rangle |_{\Delta = \Delta_{\text{spect}}}} = \frac{A^{\text{gauss}}}{A_{\text{spectr}}} = \frac{2.854}{2.25} = 1.2684 \tag{24}$$

This show that, for a given cutoff wavenumber in the inertial range, the subgrid-scale energy obtained by means of a gaussian filter is roughly 27% larger than the one obtained from a spectral filter. This was expected, since the gaussian filter is not local in the wavenumber space, differently from the spectral filter. The gaussian filter, indeed, drains also part of the energy at $\kappa \leq \kappa_c$; the scales affected by these phenomenon are called "resolved subgrid scales".

8. Consider again the sharp spectral filter. In 1980, Deardoff proposed an eddy viscosity model given by

$$\nu_{\rm sgs} = C_v \sqrt{k_{\rm sgs}} \, \Delta \tag{25}$$

Assuming equilibrium conditions and knowing that the production reads $\mathcal{P} = \nu_{\text{sgs}} |\overline{S}|^2$ with $|\overline{S}|^2 \approx 2 \int_0^{\kappa_c} \kappa^2 E(\kappa) \, d\kappa$, estimate the value of the coefficient C_v .

Solution: From step 3, we had that

$$\langle k_{\rm sgs} \rangle = \frac{3}{2} C \varepsilon^{2/3} \kappa_c^{-2/3} = \frac{3}{2} C \varepsilon^{2/3} \left(\frac{\pi}{\Delta}\right)^{-2/3}$$
 (26)

Moreover, one has

$$|\overline{S}|^2 \approx 2 \int_0^{\kappa_c} \kappa^2 E(\kappa) \, d\kappa = 2C\varepsilon^{2/3} \int_0^{\kappa_c} \kappa^2 \kappa^{-5/3} \, d\kappa = \frac{3}{2} C\varepsilon^{2/3} \left(\frac{\pi}{\Delta}\right)^{4/3}$$
 (27)

Combining the previous relations with equation (25), one obtains:

$$\mathcal{P} = \nu_{\text{sgs}} |\overline{S}|^2 = C_v \sqrt{k_{\text{sgs}}} \Delta |\overline{S}|^2 = C_v \left[\frac{3}{2} C \varepsilon^{2/3} \left(\frac{\pi}{\Delta} \right)^{-2/3} \right]^{1/2} \Delta \frac{3}{2} C \varepsilon^{2/3} \left(\frac{\pi}{\Delta} \right)^{4/3}$$
(28)

$$= C_v \left[\frac{3}{2} C \varepsilon^{2/3} \right]^{3/2} \frac{\pi}{\Delta} \Delta = C_v \left[\frac{3}{2} C \right]^{3/2} \pi \varepsilon \tag{29}$$

Under equilibrium conditions, $\mathcal{P} \approx \varepsilon$ and

$$\mathcal{P} \approx \not \in C_v \left[\frac{3}{2} C \right]^{3/2} \pi \not \in \quad \Longrightarrow \quad C_v = \frac{1}{\pi} \left[\frac{3}{2} C \right]^{-3/2} = 0.094 \tag{30}$$

9. We are now interested in applying a dynamic model, for which two filters must be defined: the "grid" filter, of width $\overline{\Delta}$, and the "test" filter, of width $\widetilde{\Delta}$, with $\widetilde{\Delta} = 2\overline{\Delta}$. Using the

Kolmogorov spectrum, estimate the ratio of the energy contained in the smallest resolved scales (i.e., the scales between $\overline{\Delta}$ and $\widetilde{\Delta}$) to the total subgrid-scale energy.

Solution: One has simply

$$r = \frac{\int_{\pi/\widetilde{\Delta}}^{\pi/\widetilde{\Delta}} C \varepsilon^{2/3} \kappa^{-5/3} \, d\kappa}{\int_{\pi/\widetilde{\Delta}}^{\infty} C \varepsilon^{2/3} \kappa^{-5/3} \, d\kappa} = \frac{\left[\frac{2}{2} \kappa^{-2/3} \right]_{\pi/\widetilde{\Delta}}^{\pi/\widetilde{\Delta}}}{\left[\frac{2}{2} \kappa^{-2/3} \right]_{\pi/\widetilde{\Delta}}^{\infty}} = \left(\frac{\widetilde{\Delta}}{\overline{\Delta}} \right)^{2/3} - 1$$
(31)

$$=2^{2/3} - 1 = 0.587\tag{32}$$

The energy contained in the smallest resolved scales corresponds to approximately 60% of the total subgrid-scale energy.

4 Hybrid Methods

4.1 DES

The Detached Eddy Simulation (DES) model initially proposed by Spalart in 1997 consists in a modification of the one-equation Spalart-Allmaras model. Specifically, the equation for the modified turbulent viscosity reads

$$\frac{\partial \nu_{\rm sa}}{\partial t} + \widetilde{u}_j \frac{\partial \nu_{\rm sa}}{\partial x_j} = c_{b1} S_{\rm sa} \nu_{\rm sa} - c_{w1} f_w^{\rm DES} \left(\frac{\nu_{\rm sa}}{d}\right)^2 + \frac{1}{\sigma} \left[\frac{\partial}{\partial x_k} \left((\widetilde{\nu} + \nu_{\rm sa}) \frac{\partial \nu_{\rm sa}}{\partial x_k}\right) + c_{b2} \frac{\partial \nu_{\rm sa}}{\partial x_k} \frac{\partial \nu_{\rm sa}}{\partial x_k}\right]$$
(1)

where the following relations hold:

$$\mu_t = \rho \nu_{\rm sa} f_{v1} \qquad S_{\rm sa} = \sqrt{2\tilde{\Omega}_{ij}\tilde{\Omega}_{ij}} + \frac{\nu_{\rm sa}}{\kappa^2 d^2} f_{v2} \qquad \tilde{\Omega}_{ij} = \frac{1}{2} \left(\frac{\partial \tilde{u}_i}{\partial x_i} - \frac{\partial \tilde{u}_j}{\partial x_i} \right)$$
 (2)

$$\chi = \frac{\nu_{\text{sa}}}{\widetilde{\nu}} \qquad f_{v1} = \frac{\chi^3}{\chi^3 + c_{v1}^3} \qquad f_{v2} = 1 - \frac{\chi}{1 + \chi f_{v1}}$$
(3)

$$f_w^{\text{DES}} = g \left(\frac{1 + c_{w3}^6}{g^6 + c_{w3}^6} \right)^{1/6} \qquad g = r + c_{w2}(r^6 - r) \qquad r^{\text{DES}} = \frac{\nu_{\text{sa}}}{S_{\text{sa}}\kappa^2 d^2}$$
 (4)

Spalart proposed to replace the d_w in r^{DES} with $d = \min(d_w, C_{\text{DES}}\Delta)$.

1. Prove that in the asymptotic limit (i.e., under the hypotheses of equilibrium and high-Re flow), $\nu_{\rm sa}$ behaves as a subgrid viscosity.

Solution: The high-Re hypothesis implies that:

• $\nu_{\rm sa}\gg\widetilde{\nu}$ because of the large turbulence activity associated to large Reynolds numbers. This implies

$$\chi \gg 1 \quad \Longrightarrow \quad f_{v1} \to 1 \quad \Longrightarrow \quad \nu_t = \nu_{\text{sa}}$$
(5)

Moreover, $f_{v2} \to 0$ and therefore $S_{sa} \approx |\Omega|$.

• $d = C_{DES}\Delta$, since the scale $d = d_w$ is recovered only close to the walls, where the high-Re assumption does not hold anymore.

On the other hand, the equilibrium condition implies that the production and dissipation are equal:

$$c_{b1}S_{sa}\nu_{sa} = c_{w1}f_w^{DES} \left(\frac{\nu_{sa}}{d}\right)^2 \tag{6}$$

Combining the two conditions, one obtains:

$$c_{b1}S_{\text{sa}}\nu_t = c_{w1}f_w^{\text{DES}} \left(\frac{\nu_t}{C_{\text{DES}}\Delta}\right)^2 \implies \nu_t = \frac{c_{b1}}{c_{w1}f_w^{\text{DES}}}C_{\text{DES}}^2\Delta^2 S_{\text{sa}}$$
 (7)

By imposing $\frac{c_{b1}}{c_{w1}f_w^{\rm DES}}C_{\rm DES}^2 = C^2$, one obtains $\nu_t = C^2\Delta^2S_{\rm sa}$ which has the same functional form of a Smagorinsky model with constant C.

4.2 Blending methods

Fan et al. in 2002 proposed a hybrid turbulence model built on a blending between a RANS and a LES model. Specifically, they considered the k_t - ω model and considered a "hybrid viscosity" and a "hybrid" turbulent kinetic energy equation defined as a weighted linear combination of the two models; that is:

$$\nu_t = \Gamma \frac{k_t}{\omega} + (1 - \Gamma)C_s \sqrt{k_t} \Delta \tag{1}$$

$$\frac{\mathrm{d}k_t}{\mathrm{d}t} = \nu_t \Omega^2 - \left[\Gamma(C_\mu k_t \omega) + (1 - \Gamma)C_d \frac{k_t^{3/2}}{\Delta} \right] + \text{diffusion}$$
 (2)

with $C_{\mu} = 0.09$, $C_s = 0.1$ and $C_d = 0.05$. The turbulence frequency ω is obtained from its own transport equation. The weighting function Γ is defined as

$$\Gamma = \tanh(\eta^4)$$
 with $\eta = \frac{1}{\omega} \max\left(\frac{\sqrt{k_t}}{C_\mu d_w}, \frac{500\nu}{d_w^2}\right)$ (3)

1. Describe the behavior of the model with respect to the weighting function Γ .

Solution: Γ explicitly depends on the inverse of the wall distance d_w . When approaching a wall, Γ increases and the model switches towards a pure k_t - ω RANS model. The max in the η definition allows to shield the viscous sublayer (since $k_t \to 0$ as $y \to 0$), keeping the RANS mode up to the wall. On the contrary, a pure LES behavior is recovered far from the walls For $\Gamma = 0$, a pure LES model is recovered; for $\Gamma = 1$, a RANS behavior is obtained.

2. Show that under the equilibrium hypothesis and in the limit $\Gamma = 0$, one obtains a Smagorinsky-type subgrid viscosity:

$$\nu_t = C_s \sqrt{\frac{C_s}{C_d}} \Delta^2 \Omega = C_F \Delta^2 \Omega \tag{4}$$

Solution: Under the equilibrium hypothesis, one has

$$\mathcal{P} = \varepsilon \quad \Longrightarrow \quad \nu_t \Omega^2 = C_d \frac{k_t^{3/2}}{\Delta} \tag{5}$$

$$C_s \sqrt{k_t} \Delta \Omega^2 = C_d \frac{k_t^{3/2}}{\Delta} \implies k_t = \frac{C_s}{C_d} \Delta^2 \Omega^2$$
 (6)

Replacing in the definition of ν_t , one has

$$\nu_t = C_s \sqrt{k_t} \Delta = C_s \sqrt{\frac{C_s}{C_d}} \Delta^2 \Omega = C_F \Delta^2 \Omega \tag{7}$$

with $C_F \approx 0.14$.

3. Under the same hypotheses, derive a one-equation model for the transport of the subgrid viscosity. Does an increase of k_t directly translate in an increasing ν_t ? Why?

Solution: Replacing k_t with ν_t , the material derivative becomes

$$\frac{\mathrm{d}k_t}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\nu_t^2}{C_s^2 \Delta^2} \right) = \frac{2\nu_t}{C_s^2 \Delta^2} \frac{\mathrm{d}\nu_t}{\mathrm{d}t}$$
 (8)

Equation (2) reads then

$$\frac{2\nu_t}{C_s^2 \Delta^2} \frac{\mathrm{d}\nu_t}{\mathrm{d}t} = \nu_t \Omega^2 - C_d \frac{k_t^{3/2}}{\Delta} \tag{9}$$

$$\frac{\mathrm{d}\nu_t}{\mathrm{d}t} = \frac{C_s^2 \Delta^2}{2} \Omega^2 - \frac{C_d C_s^2 \Delta^2}{2 \underbrace{\nu_t}{C_t \sqrt{k_t} \Delta}} \frac{k_t^{3/2}}{\Delta} = \frac{C_s^2 \Delta^2}{2} \Omega^2 - \frac{C_d C_s}{2} k_t \tag{10}$$

$$= \frac{C_s}{2} \left(C_s \Delta^2 \Omega^2 - C_d k_t \right) \tag{11}$$

The equation shows that k_t rather acts as a destruction term for ν_t , so the answer is no.

4.3 VLES

In 1998, Speziale proposed an hybrid RANS/LES method called Very Large Eddy Simulation (VLES). The main idea is to damp the Reynolds stresses in regions where the grid spacing Δ approaches the Kolmogorov scale η :

$$\tau_{ij} = \alpha \tau_{ij}^{\text{RANS}} \quad \text{with} \quad \alpha = \left[1 - \exp\left(-\frac{\beta \Delta}{\eta}\right) \right]$$
(1)

Here, β and n are some modelling parameters and $\eta = (\nu^3/\varepsilon)^{1/4}$.

1. Describe how this VLES switch from RANS to LES mode.

Solution: The RANS/LES switch is based on the Δ/η ratio. Specifically:

- For $\Delta/\eta \to 0$, $\alpha = 0 \implies \tau_{ij} = 0$. The modeled stresses are nullified and a DNS behavior is recovered;
- For $\Delta/\eta \to \infty$, $\alpha = 1 \implies \tau_{ij} = \tau_{ij}^{\text{RANS}}$. A full RANS behavior is recovered;
- For $0 < \alpha < 1$, an intermediate DNS/RANS behavior is recovered.
- 2. In your opinion, what are the strength and the weaknesses of such a model? How does it perform when turbulence is not fully developed?

Solution: Strengths:

- Any RANS eddy-viscosity model can be easily blended
- Simple and easy to implement
- The high-Reynolds asymptotic behavior is consistent with a pure RANS formulation, i.e. for $Re \to \infty \implies \eta \to 0 \implies \alpha = 1 \quad \forall \Delta$

Weaknesses:

- The DNS/RANS switch depends on the parameters β and n, which are empirical and not clearly specified
- The Kolmogorov scale η computed from the resolved flow field might not correspond to the actual η (whose value could theoretically be computed by means of DNS only)
- Recovering the correct DNS and RANS behavior for $\alpha=0$ and $\alpha=1$ does not ensure a correct LES behavior for $0<\alpha<1$

For configurations in which turbulence is not fully developed (e.g., transitional flows), the model cannot ensure a correct behavior because η is ill-defined.

3. In 2001, Magnient proposed to modify the hybrid eddy viscosity using the following form

$$\nu_t = \nu_t^{\text{RANS}} f\left(\frac{\Delta}{L_{\text{RANS}}}\right) g\left(\frac{\Delta}{\eta}\right) \tag{2}$$

and used a k_t - ε model to determine the RANS quantities. In the VLES framework, one can consider $g(\Delta/\eta) \approx 1$. Provide expressions for ν_t in the RANS and LES modes as a function of ε . Then, using the equilibrium hypothesis, provide a formulation for $f(\Delta/L_{\rm RANS})$.

Solution: From dimensional analysis, one rapidly obtains

$$\nu_t^{\rm RANS} = L_{\rm RANS}^{4/3} \varepsilon^{1/3}$$
 and $\nu_t^{\rm LES} = \Delta^{4/3} \varepsilon^{1/3}$ (3)

Under the equilibrium assumption, the kinetic energy dissipation rate is constant and therefore one has

$$\frac{\nu_t^{\text{LES}}}{\Delta^{4/3}} = \frac{\nu_t^{\text{RANS}}}{L_{\text{RANS}}^{4/3}} \tag{4}$$

Plugging this in equation (2), one obtains:

$$f\left(\frac{\Delta}{L_{\rm RANS}}\right) = \frac{\Delta^{4/3}}{L_{\rm RANS}^{4/3}} \tag{5}$$

5 PANS Modelling

The hybrid modelling RANS/LES named PANS (Partially-Averaged Navier–Stokes) has been developed by Girimaji et al. in 2005. It is based on a modified formulation of the k_t - ε turbulence model, by making it sensible to local grid refinements. In such a way, it can locally behave as a subgrid model in flow regions where the mesh has a LES-like resolution. Specifically, the PANS approach consists in introducing the unresolved-to-total ratio of kinetic energy and dissipation:

$$f_k = \frac{k_u}{k} \qquad f_\varepsilon = \frac{\varepsilon_u}{\varepsilon} \tag{1}$$

entering in the two-equation PANS model as

$$\frac{\mathrm{d}k_u}{\mathrm{d}t} = P_u - \varepsilon_u + \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{\nu_u}{\sigma_{ku}} \right) \frac{\partial k_u}{\partial x_j} \right] \tag{2}$$

$$\frac{\mathrm{d}\varepsilon_u}{\mathrm{d}t} = f_k \left(C_{\varepsilon_1} \frac{P_u \varepsilon_u}{k_u} - C_{\varepsilon_2}^* \frac{\varepsilon_u^2}{k_u} \right) + \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{\nu_u}{\sigma_{\varepsilon u}} \right) \frac{\partial \varepsilon_u}{\partial x_j} \right]$$
(3)

where P_u and ε_u are the underresolved kinetic energy production and dissipation, and $\nu_u = C_\mu \frac{k_u^2}{\varepsilon_u}$. In these equations, the coefficients $C_{\varepsilon_2}^*$, σ_{ku} and $\sigma_{\varepsilon u}$ are modified with respect the classical k_t - ε RANS model coefficients, being

$$C_{\varepsilon_2}^* \equiv C_{\varepsilon_1} + \frac{f_k}{f_{\varepsilon}} (C_{\varepsilon_2} - C_{\varepsilon_1}) \qquad \sigma_{ku} \equiv \frac{f_k^2}{f_{\varepsilon}} \sigma_k \qquad \sigma_{\varepsilon u} \equiv \frac{f_k^2}{f_{\varepsilon}} \sigma_{\varepsilon}$$
 (4)

1. Specify the interval limits of variation for the coefficients f_k and f_{ε} . For a given cutoff scale in the inertial range, which of them is bigger?

Solution: The unresolved-to-total ratio of a given quantity φ can vary between 0 (meaning that φ is completely resolved) to 1 (meaning that φ is completely unresolved, and therefore should be modelled). Hence $f_k \in [0,1]$ and $f_{\varepsilon} \in [0,1]$.

Generally, most of the kinetic energy is contained in the large scales whereas the dissipation acts mainly on the small scales. Therefore, for a given cutoff scale, one has usually that a larger portion of k is resolved with respect to ε . One can conclude that $0 \le f_k < f_{\varepsilon} \le 1$.

2. Discuss the limiting behavior of the PANS model as a function of f_k ; that is, when PANS recovers a pure RANS or a pure DNS behavior.

Solution:

• When $f_k = 1$ (and consequently also $f_{\varepsilon} = 1$), the whole k_t and ε should be modeled. In this case indeed, from equation (4) one has that $C_{\varepsilon_2}^* \equiv C_{\varepsilon_2}$, $\sigma_{ku} \equiv \sigma_k$ and $\sigma_{\varepsilon u} \equiv \sigma_{\varepsilon}$; hence, equations (2) and (3) become the classical k_t and ε equations of the pure k_t - ε RANS model. Moreover, $\nu_u = C_\mu \frac{k_u^2}{\varepsilon_u} \equiv C_\mu \frac{k_t^2}{\varepsilon} = \nu_t$.

- On the contrary, when $k_f = 0$ (and consequently, for whatever value of f_{ε}), the whole k_t should be resolved, meaning that the any model should be switched off. Indeed, the contribution of both the production and dissipation term of the dissipation equation (3) are zeroed, becoming a simple convection-diffusion equation. Furthermore, the turbulent viscosity is switched off being $\nu_u = 0$.
- 3. What would be the value of f_{ε} for a high-Reynolds flow? And for low-Reynolds one? (Assume always a cutoff in the inertial region).

Solution: For a high-Reynolds flow, the extent of the overlap between the energy-containing and dissipation ranges tend to zero, thus we would have $f_{\varepsilon} = 1$. On the contrary, for a low-Reynolds flow the two ranges tend to be superposed, hence $f_{\varepsilon} \approx f_k$.

4. In this model, it would be convenient to find an estimation for the lowest value of f_k that a given grid of grid size Δ could support at a given location. Show that one has:

$$f_k = \min \left[1, \frac{1}{\sqrt{C_\mu}} \left(\frac{\Delta}{L_T} \right)^{2/3} \right] \tag{5}$$

where $L_T = \frac{k_t^{3/2}}{\varepsilon}$ is the local Taylor turbulent scale. To do this, assume that $f_{\varepsilon} = 1$, and

that the smallest resolved length scale η_r can be computed as $\eta_r = \left[\frac{\nu_u^3}{\varepsilon}\right]^{\frac{1}{4}}$.

Solution: Since $k_t = f_k k_u$ and $\varepsilon = f_{\varepsilon} \varepsilon_u = \varepsilon_u$ (f_{ε} being 1), one has that

$$\nu_u = C_\mu \frac{k_u^2}{\varepsilon_u} = C_\mu f_k^2 \frac{k_t^2}{\varepsilon} \tag{6}$$

A typical guideline in DNS is that the grid size Δ should be of the order of the Kolmogorov length-scale η_k . Similarly for PANS, one has that Δ should be similar to the smallest resolved scale η_r . Thus:

$$\eta_r = \left[\frac{\nu_u^3}{\varepsilon}\right]^{\frac{1}{4}} = \left[\frac{\left(C_\mu f_k^2 \frac{k^2}{\varepsilon}\right)^3}{\varepsilon}\right]^{\frac{1}{4}} = C_\mu^{\frac{3}{4}} f_k^{\frac{3}{2}} \frac{k_t^{3/2}}{\varepsilon} = C_\mu^{\frac{3}{4}} f_k^{\frac{3}{2}} L_T \approx \Delta \tag{7}$$

Rearranging the relation, one obtains

$$f_k = \frac{1}{\sqrt{C_\mu}} \left[\frac{\Delta}{L_T} \right]^{2/3} \tag{8}$$

Recalling that the value of f_k cannot exceed unity, the two conditions can be assembled to obtain:

$$f_k = \min\left[1, \frac{1}{\sqrt{C_\mu}} \left(\frac{\Delta}{L_T}\right)^{2/3}\right] \tag{9}$$