1 The stretched-spiral vortex subgrid-scale model for large-eddy simulation

These draft notes are to accompany the C code `spiral.[ch]` that implements the stretched-spiral vortex subgrid-scale model for large-eddy simulation developed by Pullin *et al.* at the Graduate Aerospace Laboratories the California Institute of Technology <fluids.caltech.edu>.

We kindly ask you to acknowledge any of the relevant papers from the research group, listed at the end of this document, if the code is used in any program or if its use leads to any publications.

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2.1 Filtered Navier–Stokes equations

Define the LES filter G associated with cutoff scale Δ_c,

$$\overline{\phi}(\boldsymbol{x}) = \int G(\boldsymbol{x} - \boldsymbol{x}'; \Delta_c)\phi(\boldsymbol{x}')\,\mathrm{d}\boldsymbol{x}'.$$

Typically, $\Delta_c = (\Delta x\,\Delta y\,\Delta z)^{1/3}$. Applying the filter G to the Navier–Stokes equations, we obtain the equations for large-eddy simulation (LES) [12]:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u}_j}{\partial x_j} = 0,$$

$$\frac{\partial \overline{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial \left(\overline{\rho}\widetilde{u}_i\widetilde{u}_j + \overline{p}\delta_{ij} - d_{ij} + \overline{\rho}T_{ij}\right)}{\partial x_j} = 0,$$

$$\frac{\partial \overline{\rho}\widetilde{\psi}}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{\psi}\widetilde{u}_j + D\overline{\rho}\frac{\partial \widetilde{\psi}}{\partial x_j} + \overline{\rho}q_j\right) = 0,$$

where

$$T_{ij} = \widetilde{u_i u_j} - \widetilde{u}_i\,\widetilde{u}_j, \quad q_j = \widetilde{\psi u_j} - \widetilde{\psi}\,\widetilde{u}_j$$

are unclosed subgrid-scale (SGS) terms to be modeled. d_{ij} is the deviatoric Newtonian stress tensor; ψ is a scalar.

2.2 The stretched-spiral vortex subgrid-scale model

The stretched-spiral vortex [1] is a physical model for turbulent fine scales where the flow is composed of an ensemble of tube-like structures with concentrated vorticity. On a segment of such tubes, the flow is approximated by an axially-stretched two-dimensional flow. These simplified equations admit analytical large-time asymptotic solutions, from which ensemble statistics, such as correlation and spectra, follows. These have been studied extensively and were found to be consistent with experimental data [1, 2, 3, 4, 5, 6, 7].

[8, 9, 10, 11, 12, 13, 14] used the stretched-spiral vortex to model SGS motion for LES in the following way. Embedded in each computational cell it is assumed that there exists a superposition of stretched-spiral vortices, each having orientation taken from a probability density function (p.d.f.), $P(\alpha,\beta)$, where α and β are Euler angles relative to the laboratory frame. Assuming that the SGS ensemble dynamics can be characterized by a single vortex described by the particular Euler angles α_0 and β_0, the orientation p.d.f. is then modeled with delta functions,

$$P(\alpha,\beta) = \frac{4\pi}{\sin\alpha_0}\delta(\alpha-\alpha_0)\delta(\beta-\beta_0).$$

We write α_0 and β_0 in terms of the unit vector of the vortex axis $\boldsymbol{e}^v$,

$$e_1^v = \sin\alpha_0\cos\beta_0, \quad e_2^v = \sin\alpha_0\sin\beta_0, \quad e_3^v = \cos\alpha_0.$$

The resulting SGS stress tensor of the ensemble described by the orientation p.d.f. is [4, 8]

$$T_{ij} = (\delta_{ij} - e_i^v e_j^v)K,$$

where K is the SGS kinetic energy, given by

$$K = \int_{k_c}^{\infty} E(k)\,\mathrm{d}k, \tag{2.1}$$

where $k_c = \pi/\Delta_c$, the cutoff wavenumber; $E(k)$ is the SGS energy spectrum.

The above is essentially kinematical and is independent of the detailed subgrid vortex dynamics [4]. If it is further assumed that the SGS vortices are of the stretched-spiral type, which have energy spectra, determined by detailed Navier–Stokes dynamics, of the form [1]

$$E(k) = \mathcal{K}_0 \epsilon^{2/3} k^{-5/3} \mathrm{e}^{-k^2 \lambda_v^2}, \tag{2.2}$$

where $\lambda_v^2 = 2\nu/(3|\widetilde{a}|)$; $\widetilde{a} = e_i^v e_j^v \widetilde{S_{ij}}$, the stretching along the SGS vortex axis imposed by resolved scales; and $\widetilde{S_{ij}} = (\partial \widetilde{u_i}/\partial x_j + \partial \widetilde{u_j}/\partial x_i)/2$, the resolved strain-rate tensor, then combining (2.1) and (2.2), we obtain

$$K = \mathcal{K}_0 \epsilon^{2/3} k_c^{-2/3} P(k_c \lambda_v) \tag{2.3}$$

where

$$P(\kappa_c) = \frac{1}{2} \kappa_c^{2/3} \Gamma_{-1/3}(\kappa_c^2), \tag{2.4}$$

$\Gamma_{-1/3}$ is an incomplete gamma function.

Following [9], the grouped constant $\mathcal{K}_0 \epsilon^{2/3}$ is determined from the following procedure: calculate the local average of the resolved-scale second-order structure function from the LES simulation and match it to the stretched-spiral vortex prediction for the same grouped constant. This matching procedure provides, except for the choice of vortex alignment $\boldsymbol{e}^v$, a parameter-free SGS model.

Past choices of the local averaging region used for the match were the circle and spherical shell, (19) and (A2) in [9]. We generalize these by applying to the structure function match, (18) in [9], an average in $\boldsymbol{x}'$, denoted by $\langle\ \rangle$, over an arbitrary domain:

$$\langle F_2 \rangle = \left\langle 4 \int_0^{k_c} E(k) \left[1 - J_0(kr)\right] \mathrm{d}k \right\rangle, \tag{2.5}$$

where F_2 is the local second-order structure function as calculated from the running simulation,

$$F_2 = [\delta \widetilde{u_i}]^2 = [\widetilde{u_i}(\boldsymbol{x}) - \widetilde{u_i}(\boldsymbol{x}')]^2, \quad r^2 = (|\delta \boldsymbol{x}|)^2 - (\delta \boldsymbol{x} \cdot \boldsymbol{e}^v)^2, \quad \delta \boldsymbol{x} = \boldsymbol{x} - \boldsymbol{x}'.$$

Here, $\boldsymbol{x}'$ is the integration variable; J_0 is the zeroth-order Bessel function of the first kind; and r is the distance from $\boldsymbol{x}'$ to the vortex axis. Substituting the energy spectrum, (2.2) into (2.5), and simplifying, we find that

$$\mathcal{K}_0 \epsilon^{2/3} k_c^{-2/3} = \frac{\langle F_2 \rangle}{\langle Q(k_c \lambda_v, d) \rangle}, \tag{2.6}$$

where

$$Q(\kappa_c, d) = 4 \kappa_c^{2/3} \int_0^{\kappa_c} \kappa^{-5/3} \mathrm{e}^{-\kappa^2} [1 - J_0((\kappa/\kappa_c)\pi d)] \, \mathrm{d}\kappa, \quad d = r/\Delta_c. \tag{2.7}$$

Combining (2.3), (2.4), (2.6), and (2.7), we have

$$K = \frac{\langle F_2 \rangle}{\langle Q(k_c \lambda_v, d) \rangle} P(k_c \lambda_v).$$

Computationally efficient approximations for $P(\kappa_c)$ and $Q(\kappa_c, d)$ are provided below.

We now choose the averaging operator to be the ensemble (discrete) average

$$\langle \phi \rangle = \frac{1}{N} \sum_{\boldsymbol{x}' \in \mathcal{N}(\boldsymbol{x})} \phi,$$

where ϕ is either F_2 or Q, $\mathcal{N}(\boldsymbol{x})$ is the set of all points near $\boldsymbol{x}$, and N is the number of points in $\mathcal{N}(\boldsymbol{x})$. Note that here, the ensemble average is applied on both F_2 and Q, while [9] applied the ensemble average on F_2, but used its continuous analog on Q. The approach taken here allows the domain of averaging, $\mathcal{N}(\boldsymbol{x})$, to be quite general and can be adapted for unstructured meshes. For a structured Cartesian grid, a convenient choice is $\mathcal{N}(\boldsymbol{x})$ consisting of points within the closed $(2\Delta x) \times (2\Delta y) \times (2\Delta z)$ block centred on $\boldsymbol{x}$, that is,

$$\mathcal{N}(\boldsymbol{x}) = \{\boldsymbol{x}' : \boldsymbol{x}' \neq \boldsymbol{x}, |x - x'| \leq \Delta_x, |y - y'| \leq \Delta_y, |z - z'| \leq \Delta_z\};$$

correspondingly, $N = 3^3 - 1 = 26$.

2.3 Scalar flux model

The scalar flux that models the convective transport of scalar by SGS vortices is given by [10]:

$$q_i = -\gamma \frac{\Delta_c}{2} K^{1/2} (\delta_{ij} - e_i^v e_j^v) \frac{\partial \widetilde{\psi}}{\partial x_j},$$

where $\gamma = 1$, a universal model constant.

3 Numerical implementation

3.1 Structure function integral

This is similar to the appendix given by [9]. We seek a computationally efficient approximation to the integral (2.5)

$$Q(\kappa_c, d) = 4\kappa_c^{2/3} \int_0^{\kappa_c} \kappa^{-5/3} \mathrm{e}^{-\kappa^2} [1 - J_0((\kappa/\kappa_c)\pi d)] \, \mathrm{d}\kappa.$$

We are only interested in accurately approximating Q in the high Reynolds number regime, represented by the limit $\kappa_c = k_c \lambda_v \ll 1$. Perform the change of variables, $\kappa/\kappa_c = \xi$,

$$
\begin{aligned}
Q(\kappa_c, d) &= 4\int_0^1 \xi^{-5/3} \mathrm{e}^{-\xi^2\kappa_c^2}[1 - J_0(\xi\pi d)]\,\mathrm{d}\xi \\
&\sim 4\int_0^1 \xi^{-5/3}[1 - J_0(\xi\pi d)]\,\mathrm{d}\xi
\end{aligned}
$$

for $\kappa_c \ll 1$. Expanding Q:

$$
\begin{aligned}
Q(\kappa_c, d) &= 4\int_0^1 \xi^{-5/3}[1 - J_0(\xi\pi d)]\,\mathrm{d}\xi \\
&= 4\int_0^\infty \xi^{-5/3}[1 - J_0(\xi\pi d)]\,\mathrm{d}\xi - 4\int_1^\infty \xi^{-5/3}\,\mathrm{d}\xi + 4\int_1^\infty J_0(\xi\pi d)\,\mathrm{d}\xi \\
&= 3(\pi d)^{2/3}\pi^{1/2}(\Gamma_{7/6})^{-1} - 6 + 4\int_1^\infty J_0(\xi\pi d)\,\mathrm{d}\xi
\end{aligned}
$$

For the last integral, replace the Bessel function with its large asymptotic expansion for large argument, and integrate by parts once to obtain the leading order term:

$$
4\int_1^\infty J_0(\xi\pi d)\,\mathrm{d}\xi \sim -4\sqrt{2/\pi}(\pi d)^{-3/2}\sin(\pi d - \pi/4)
$$

for $d \gg 1$. Put all together:

$$
\begin{aligned}
Q(\kappa_c, d) &\sim 3(\pi d)^{2/3}\pi^{1/2}(\Gamma_{7/6})^{-1} - 6 - 4\sqrt{2/\pi}(\pi d)^{-3/2}\sin(\pi d - \pi/4) \\
&\sim 12.2946\, d^{2/3} - 6 - 0.573159\, d^{-3/2}\sin(\pi d - \pi/4).
\end{aligned}
$$

for $\kappa_c \gg 1$ and $d \gg 1$ with relative error of 2.71% at $d = 0.873469$. For $d \ll 1$, expand the Bessel function, $1 - J_0(\xi\pi d) \sim (\xi\pi d)^2/4 - (\xi\pi d)^4/64$:

$$
\begin{aligned}
Q(\kappa_c, d) &\sim (\pi d)^2\int_0^1 \xi^{1/3}\,\mathrm{d}\xi - (\pi d)^4/16\int_0^1 \xi^{7/3}\,\mathrm{d}\xi \\
&\sim (3/4)(\pi d)^2 - (3/160)(\pi d)^4 \sim 7.4022d^2 - 1.82642d^4.
\end{aligned}
$$

with relative error 2.71% at $d = 0.873469$. We numerically approximate $Q(\kappa_c, d)$ in two pieces: one for small d and another for large d matching at $d = 0.873469$.

3.2 Spherical average

If the averaging domain has spherical symmetry, we can average over a spherical shell of normalized radius d_0 to obtain

$$
Q^s(\kappa_c, d_0) = \frac{1}{4\pi d_0^2}\int_0^\pi\int_0^{2\pi} Q(\kappa_c, d_0\sin\theta)d_0^2\sin\theta\,\mathrm{d}\phi\,\mathrm{d}\theta
$$

and for $\kappa_c \to 0$ and $d_0 = 1$

$$\begin{aligned} Q^s(\kappa_c, d_0) &= \frac{1}{4\pi} \int_0^{\pi} \int_0^{2\pi} 4 \int_0^1 \xi^{-5/3} [1 - J_0(\xi \pi d_0 \sin\theta)] \, \mathrm{d}\xi \sin\theta \, \mathrm{d}\phi \, \mathrm{d}\theta \\ &= 4 \int_0^1 \xi^{-5/3} \left(1 - \frac{\sin(\xi \pi d_0)}{\xi \pi d_0} \right) \mathrm{d}\xi \approx 4.09047 = 1.90695\pi^{2/3}, \end{aligned}$$

which is $A\pi^{2/3}$ in (6) of [10].

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