Computer Physics Communications 184 (2013) 2651–2661

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

Large-eddy simulation of hypersonic flows. Selective procedure to activate the sub-grid model wherever small scale turbulence is present

D. Tordella [a,*], M. Iovieno [a], S. Massaglia [b], A. Mignone [b]

[a] *Politecnico di Torino, Dipartimento di Ingegneria Meccanica e Aerospaziale, Corso Duca degli Abruzzi 24, 10129 Torino, Italy*

[b] *Università di Torino, Dipartimento di Fisica Generale, via P.Giuria 1, 10125 Torino, Italy*

ARTICLE INFO

Article history:
Received 8 August 2012
Received in revised form
26 April 2013
Accepted 10 June 2013
Available online 4 July 2013

Keywords:
Small scale
Turbulence
Localization
Large-eddy simulation
Astrophysical jets

ABSTRACT

A new method for the localization of the regions where small scale turbulent fluctuations are present in hypersonic flows is applied to the large-eddy simulation (LES) of a compressible turbulent jet with an initial Mach number equal to 5. The localization method used is called selective LES and is based on the exploitation of a scalar probe function f which represents the magnitude of the *stretching–tilting* term of the vorticity equation normalized with the enstrophy (Tordella et al., 2007) [3]. For a fully developed turbulent field of fluctuations, statistical analysis shows that the probability that f is larger than 2 is almost zero, and, for any given threshold, it is larger if the flow is under-resolved. By computing the spatial field of f in each instantaneous realization of the simulation it is possible to locate the regions where the magnitude of the normalized vortical stretching–tilting is anomalously high. The sub-grid model is then introduced into the governing equations in such regions only. The results of the selective LES simulation are compared with those of a standard LES, where the sub-grid terms are used in the whole domain, and with those of a standard Euler simulation with the same resolution. The comparison is carried out by assuming as reference field a higher resolution Euler simulation of the same jet. It is shown that the *selective* LES modifies the dynamic properties of the flow to a lesser extent with respect to the classical LES. In particular, the prediction of the enstrophy, mean velocity and density distributions and of the energy and density spectra are substantially improved.

1. Introduction: the small scale detection criterion

Turbulent flows in many different physical and engineering applications have a Reynolds number so high that a direct numerical simulation of the Navier–Stokes equations (DNS) is not feasible. The large-eddy simulation (LES) is a method in which the large scales of turbulence only are directly solved while the effects of the small-scale motions are modelled. The mass, momentum and energy equations are filtered in space in order to obtain the governing equation for the large scale motions. The momentum and energy transport at the large-scale level due to the unresolved scales is represented by the so-called subgrid terms. Standard models for such terms, as, for example, the widely used Smagorinsky model, are based on the assumption that the unresolved scales are present in the whole domain and that turbulence is in equilibrium at subgrid scales (see, e.g., [1,2]). This hypothesis can be questionable in free, transitional and highly compressible turbulent flows where subgrid scales, that is fluctuations on a scale smaller than the space filter size, are not simultaneously present in the whole domain. In such situations, subgrid models such as Smagorinsky's overestimate the energy flow toward subgrid scales and, from the point of view of the large, resolved, scales, they appear as over-dissipative by exceedingly damping the large-scale motion.

For instance, simulation of astrophysical jets could suffer from such limitation. In this regard, any improvement of the LES methodology is opportune. Astrophysical flows occur in very large sets of spatial scales and velocities, are highly compressible (Mach number up to 10^2) and have a Reynolds number which can exceed 10^{13}, so that only the largest scales of the flow can be resolved even by the largest simulation in the foreseeable future. As a consequence, today, in this field, LES appears as a feasible simulation method able to predict the unsteady system behaviour.

We have recently proposed a simple method to localize the regions where the flow is underresolved [3]. The criterion is based on the introduction of a local functional of vorticity and velocity gradients. The regions where the fluctuations are unresolved are located by means of the scalar probe function [3] which is based

* Corresponding author. Tel.: +39 011 0906812; fax: +39 011 090 6899.
E-mail address: daniela.tordella@polito.it (D. Tordella).

0010-4655/$ – see front matter © 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.cpc.2013.06.012

on the vortical stretching–tilting sensor:

$$f(\mathbf{u}, \boldsymbol{\omega}) = \frac{|(\boldsymbol{\omega} - \overline{\boldsymbol{\omega}}) \cdot \nabla(\mathbf{u} - \overline{\mathbf{u}})|}{|\boldsymbol{\omega} - \overline{\boldsymbol{\omega}}|^2} \tag{1}$$

where $\mathbf{u}$ is the velocity vector, $\boldsymbol{\omega} = \nabla \times \mathbf{u}$ is the vorticity vector and the overbar indicates the statistical average. Function (1) is a normalized scalar form of the vortex-stretching term that represents the inertial generation of three dimensional vortical small scales inside the vorticity equation. When the flow is three dimensional and rich in small scales f is necessarily different from zero, while, on the other hand, it is instead equal to zero in a two-dimensional vortical flow where the vortical stretching is absent. The mean flow is subtracted from the velocity and vorticity fields in order to consider the fluctuating part of the field only.

A priori test of the spatial distribution of functional test have been performed by computing the statistical distribution of f in a fully resolved turbulent fluctuation field (DNS of a homogeneous and isotropic turbulent flow (1024^3, $Re_\lambda = 230$, data from [4])) and in some unresolved instances obtained by filtering this DNS field on coarser grids (from 512^3 to 64^3). It has been shown [3] that the probability that f assumes values larger than a given threshold t_ω is always higher in the filtered fields and increases when the resolution is reduced. The difference between the probabilities in fully resolved and in filtered turbulence is maximum when t_ω is in the range [0.4, 0.5] for all resolutions. In such a range the probability $p(f \geq t_\omega)$ that f is larger than t_ω in the less resolved field is about twice the probability in the DNS field. Furthermore, beyond this range this probability normalized over that of resolved DNS fields it is gradually increasing becoming infinitely larger. From that it is possible to introduce a threshold t_ω on the values of f, such that, when f assumes larger values the field could be considered locally unresolved and should benefit from the local activation of the Large Eddy Simulation method (LES) by inserting a subgrid scale term in the motion equation. The values of this threshold is arbitrary, as there is no sharp cut, but it can be reasonably chosen as the one which gives the maximum difference between the probability $p(f \geq t_\omega)$ in the resolved and unresolved fields. This leads to $t_\omega \approx 0.4$. Furthermore, it should be noted that the Morkovin hypothesis, stating that the compressibility effects do not have much influence on the turbulence dynamics, apart from varying the local fluid properties [5], allows to apply the same value of the threshold in compressible and incompressible flows.

Such value of the threshold has been used to investigate the presence of regions with anomalously high values of the functional f, by performing a set of a priori tests on existing Euler simulations of the temporal evolution of a perturbed cylindrical hypersonic light jet with an initial Mach number equal to 5 and ten times lighter than the surrounding external ambient [3]. When the effect of the introduction of subgrid scale terms in the transport equation is extrapolated from those a priori tests, they positively compare with experimental results and show the convenience of the use of such a procedure [3,6,7].

In this paper we present large-eddy simulations of this temporal evolving jet, where the subgrid terms are selectively introduced in the transport equations by means of the local stretching criterion [3]. The aim is not to model a specific jet, but instead to understand, from a physical point of view, the differences introduced by the presence of sub-grid terms in the under-resolved simulations of hypersonic jets.

Our localization procedure selects the regions where subgrid terms are applied and, as such, its effect could be considered equivalent to a model coefficient modulation, as the one obtained by the dynamic procedure [8] or by the use of improved eddy viscosity Smagorinsky-like models like Vreman's model [9], which gives a low eddy viscosity in non turbulent regions of the flow. However, it operates differently because it is completely uncoupled from the subgrid scale model used as, unlike the common practical implementations of the dynamic procedure, does not require ensemble averaging to prevent unstable eddy viscosity. Other alternatives, such as the approximate deconvolution model [10], are more complicated than the present selective procedure because involve filter inversion and the use of a dynamic relaxation term. The computational overload of the selective filtering is modest and can make LES an affordable alternative to a higher resolution inviscid simulation: the selective LES increases the computing time of about one-third with respect to an Euler simulation, while the doubling of the resolution can increase the computing time by a factor of sixteen.

2. Flow configuration and the numerical method

We have simulated the temporal evolution of a three dimensional jet in a parallelepiped domain with periodicity conditions along the longitudinal direction. The flow is governed by the ideal fluid equations (mono-atomic gas flow) for mass, momentum, and energy conservation. The beam is considered thermally confined by the external medium, and the initial pressure is set uniform in the entire domain. In the astrophysical context, this formulation is usually considered to approximate the temporal hydrodynamic evolution inside a spatial window of interstellar jets, which are highly compressible collimated jets characterized by Reynolds numbers of the order 10^{10-15}. See for example, the Herbig–Haro jets HH24, HH34 and HH47 [11,12]. We do not consider the effect of the radiative cooling, which can change the jet dynamics substantially (see, e.g. [13,14]). The transient evolution includes basically two principal mechanism, the growth and evolution of internal shocks and the dynamics of the mixing process originated by the nonlinear development of the Kelvin Helmholtz instability. The analysis is carried out through hydro-dynamical simulations by considering only a fraction of the beam which is far from its base and head. Due to the use of the periodic boundary conditions, the jet material is continually processed by the earlier evolution because of the multiple transits though the computational domain. In this way, the focus is put on the instability evolution and on the interaction between the jet and the external medium, rather than an analysis of the global evolution of the jet.

It is known that the numerical solution of a system of ideal conservation laws (such as the Euler equations) actually produces the equivalent solution of another modified system with additional diffusion terms. With the discretizations used in this study it possible to estimate *a posteriori* that the numerical viscosity implies an actual Reynolds number of about 10^3. In such a situation it is clear that the addition into the governing equations of the diffusive–dissipative terms relevant to a Reynolds number in the range 10^{10-15} would be meaningless. The formulation used is thus the following:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}\left(\rho u_i\right) = 0 \tag{2}$$

$$\frac{\partial(\rho u_k)}{\partial t} + \frac{\partial}{\partial x_i}\left(\rho u_i u_k + p\delta_{ik}\right) = \frac{\partial}{\partial x_i} H\left(f_{\rm LES} - t_\omega\right) \tau_{ik}^{SGS} \tag{3}$$

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_i}\left[(E+p)u_i\right] = \frac{\partial}{\partial x_i} H(f_{\rm LES} - t_\omega) q_i^{SGS} \tag{4}$$

where the field variables p, ρ and u_i and E are the filtered pressure, density, velocity, and total energy respectively. The ratio of specific heats γ is equal to 5/3. Here τ_{ik}^{SGS} and q_i^{SGS} are the subgrid stress tensor and total enthalpy flow, respectively. Function $H(\cdot)$ is the Heaviside step function, thus the subgrid scale fluxes are applied only in the regions where $f > t_\omega$. The threshold t_ω is here taken equal to 0.4, which is the value for which the maximum