Physical scaling of numerical dissipation for LES

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1 Introduction

In this work, we are interested in an alternative way to perform LES using a numerical substitute of a subgrid-scale model with a calibration based on physical inputs. This approach can be seen as falling within Implicit LES (ILES) because it is based on an artificial dissipation operator where the numerical error is the source of the regularization. However, the purpose here is to control explicitly this error to enable it to play the role of an explicit subgrid-scale model.

The most popular ILES are based on differentiation operators that introduce artificial dissipation in order to mimic the dissipative mechanisms of the subgrid-scales. For this ILES family, the term "implicit" can be understood in the sense that the actual equations to be solved are the Navier-Stokes equations without any extra explicit modelling as in a DNS. In practice, the numerical dissipation provided by some specific schemes (typically upwind schemes) can act at small-scales in a manner similar to an explicit subgrid-scale model. This favourable property, sometimes referred to as the "convenient conspiracy", does not hold systematically because a scheme that provides an acceptable artificial dissipation at one spatial resolution can become sub- or over-dissipative at another resolution. That is why some authors have developed different versions of their schemes depending on their ILES resolution. The goal of the present study is to examine how this weakness can be overcome through flexible and accurate numerics with physical inputs.

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2 General methodology and goal

Here, we present an ILES modelling where the artificial dissipation is introduced by the molecular dissipation operator, namely the viscous term [5]. As for standard ILES, the source of artificial dissipation is the numerical error. However, an originality of the approach is that it is based on high-order centred finite-difference schemes for the computation of the second derivatives in the Navier-Stokes equations. Importantly, these schemes are implicit in space (they are often referred to as "compact", see [6] for a comprehensive presentation) thereby enabling flexibility for the control of their artificial dissipative features. It can be easily shown that the use of a finite difference scheme with a modified square wavenumber k'' that overestimates its exact counterpart k^2 is equivalent to the introduction of a spectral viscosity $\nu_s(k)$ given by $\nu_s(k) = \nu\frac{k''(k)-k^2}{k^2}$ where ν is the kinematic molecular viscosity. The flexibility to shape k'' makes it possible to prescribe any value ν_0 to the spectral viscosity at the cutoff wavenumber $k_c = \pi/\Delta x$ while at the same time controlling the kernel $\nu_s(k)/\nu_0$ (Δx is the mesh size). For instance, [5] have used this flexibility to mimic the Spectral Vanishing Viscosity (SVV) or hyperviscous kernels while ensuring high-order accuracy.

The first calculations based on this approach have been successful for DNS as well as for LES. For the former, a moderate value of ν_0 with a very selective kernel concentrated near k_c is helpful to control spurious oscillations due to aliasing. For the latter, after the successful calculation of a turbulent channel flow by [5], [2] have shown that this kind of implicit subgrid-modelling drastically improves the prediction of heat transfer for an impinging jet flow compared to eddy viscosity subgrid-scale closures such as the dynamic Smagorinsky or the WALE models.

Even if these first LES results are encouraging, the flexibility in the prescription of $\nu_s(k)$ can also be seen as a drawback because of the arbitrariness introduced by the need to chose both ν_0 and the kernel $\nu_s(k)/\nu_0$ appropriately case by case. The aim of this study is therefore to provide ways to constrain this choice by appropriate physical scaling of the numerical dissipation. To predict the value of ν_0 required for a given LES spatial resolution, we propose an approach based on the solution of a Pao-like equation. The method is validated on DNS and LES of the 3D Taylor-Green vortex problem.

3 Pao-like solution

In the framework of homogeneous and isotropic turbulence, and assuming that a spectral range exists where the energy spectrum is stationary[1], the Lin equation leads to

[1] Note, however, that evidence has been accumulating over the past 8 years which shows that there is no significant such range except perhaps in the directly viscous dissipation range, see [3] and references therein, but the present work is only a starting point which will evolve accordingly

$$T(k) = 2\nu k^2 E(k) \tag{1}$$

where $E(k)$ is the kinetic energy spectrum whereas $T(k)$ is the transfer term related to the energy flux $\Pi(k)$ by $-d\Pi(k)/dk = T(k)$. As in the Kolmogorov theory, this flux can be assumed to depend only on the dissipation ε and the wavenumber k. Then, for dimensional reasons, equation (1) becomes

$$\frac{d}{dk}\left(1/C_k\varepsilon^{1/3}k^{5/3}E(k)\right) + 2\nu k^2 E(k) = 0 \tag{2}$$

with the analytical solution

$$E(k) = C_k\varepsilon^{2/3}k^{-5/3}\exp\left(-3/2C_k\left(k/k_\eta\right)^{4/3}\right) \tag{3}$$

where $k_\eta = \varepsilon^{1/4}/\nu^{3/4}$ is the Kolmogorov wavenumber (see [7] for more details).

As a tool to predict the spectrum that should be obtained by the present type of LES, a similar approach can be used by replacing k^2 on the right hand side of equation (2) with k''. Then, the resulting differential equation can be solved numerically in a spectral range between a wavenumber k_s (below which $\nu_s(k)$ is assumed to vanish) and infinity. This computationally inexpensive solution can be done for any value of ν_0 leading to a set of Pao-like solutions.

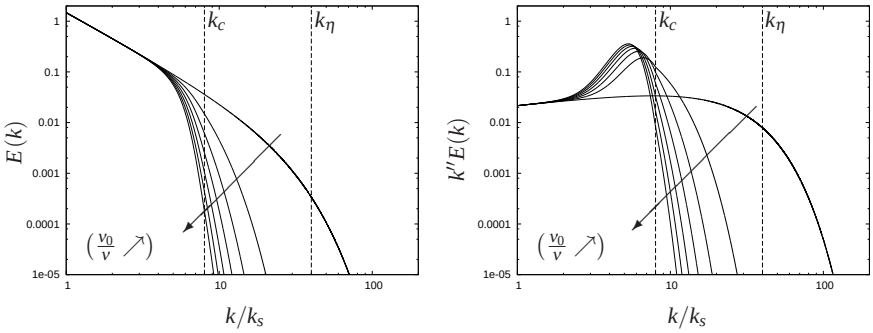

Fig. 1 Kinetic energy $E(k)$ and dissipation $k''E(k)$ spectra obtained by solving the Pao-like equation from $\nu_0/\nu = 0$ (reference Pao solution) to $\nu_0/\nu = 48$ by steps of 8.

To illustrate the behaviour of such Pao-like solutions, the case $k_\eta/k_c = 5$ is considered with a SVV-like kernel (plotted in figure 2-left). First, it is interesting to investigate how the increase of ν_0/ν modifies the kinetic energy spectrum and its related dissipation spectrum (including the numerical contribution). Six kinetic energy spectra are presented in figure 1-left. The reference spectrum corresponds to the case $\nu_0/\nu = 0$ for which the Pao spectrum (3) is virtually recovered. Then, ν_0/ν is increased by steps of 8 up to the value 48. As ν_0/ν is increased, the overall range of the predicted spectrum is reduced. For the highest values of ν_0/ν, this reduction corresponds to a strong fall at the cutoff wavenumber $k_c = 8k_s$ considered for this ex-

ample. The resulting low levels of $E(k_c)$ suggest that the corresponding LES could be done using a mesh such as $\Delta x = \pi/k_c$. For instance, to have the same kinetic energy at k_c as at k_η for the reference DNS (for which $\nu_0/\nu = 0$), a simple dichotomic search provides the value $\nu_0/\nu = 42.37$. Using the Pao-like solver, this dichotomic search ensuring $E_{LES}(k_c) = E_{DNS}(k_\eta)$ can be performed extensively for any ratio k_η/k_c. Figure 2-right presents the resulting behaviour for the range $1 \leq k_\eta/k_c \leq 30$. As expected, the Sharp SVV kernel (plotted in figure 2-left) requires to use significantly higher values of ν_0/ν (see figure 2-right).

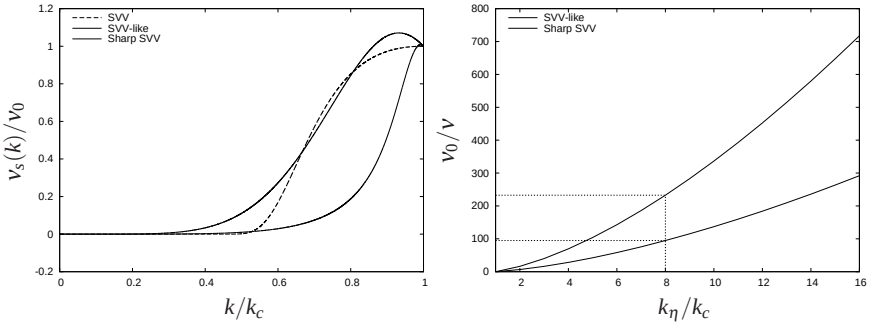

Fig. 2 Left: SVV-like and Sharp SVV kernels. Right: evolution of ν_0/ν with k_η/k_c to ensure $E_{LES}(k_c) = E_{DNS}(k_\eta)$ as predicted by the Pao-like solution.

The corresponding dissipation spectra (figure 1-right) clearly show how the use of high-order numerical viscosity can concentrate an extra-dissipation near k_c in order to compensate the lack of dissipation for $k > k_c$ (which could not be taken into account using a discretization based on mesh size with $\Delta x = \pi/k_c$).

4 DNS and LES results

The suitability of the present prediction of ν_0/ν is examined by performing LES of the 3D Taylor-Green vortex problem while using filtered DNS results as reference for comparison (case "DNS$_f$"). Both DNS and LES are carried out using the high-order flow solver "Incompact3d" which is based on sixth-order finite-difference schemes [4]. For the sake of clarity, only the Reynolds number $Re = 5000$ is presented here. For this fairly high value, accurate DNS results can be obtained with a regular Cartesian mesh of 1280^3 mesh odes on a triperiodic domain $2\pi^3$. For the present calculations, using the symmetries of the problem, only the flow inside the impermeable box π^3 is explicitly calculated with a reduction of the computational cost by a factor 8. Then, comparable LES are performed using 160^3 mesh nodes with $k_\eta/k_c = 8$ which represents a reduction of the computational cost by a factor of 4096 by comparison with DNS. The Pao-like solver provides the values $\nu_0/\nu \approx 95$ and 232 for the SVV-like and Sharp SVV kernels respectively (see figure 2-right).

When these values are used in the present type of LES, satisfactory results are obtained with a clear improvement compared to a calculation performed at the same spatial resolution but free from subgrid-scale modelling and artificial dissipation. This improvement can be illustrated by considering the time evolution of the kinetic energy E_k and its dissipation $\varepsilon = -dE_k/dt$ (that includes the numerical contribution) as presented in figure 3 (left). The filtered DNS data are obtained after the application of the filter $T_f(k) = \sqrt{E_{LES}(k)/E_{DNS}(k)}$ in the Fourier space where $E_{DNS}(k)$ is the Pao kinetic energy spectrum whereas $E_{LES}(k)$ is its Pao-like counterpart for a given set of ν_0 and kernel $\nu_s(k)/\nu_0$. Here, for the sake of brevity, only the Sharp SVV kernel is considered with $\nu_0/\nu = 232$.

The calculation free from extra dissipation, referred to as "LES no model" case, means that a conventional compact finite difference scheme is used to compute the viscous term. Interestingly, although this configuration is *a priori* sub-dissipative, an over-dissipative behaviour seems to be observed *a posteriori* throughout the calculation as shown in figure 3 (left). A close examination of the time evolution of E_k and ε reveals that in fact, the "LES no model" case is very slightly sub-dissipative just a the beginning of the simulation. This lack of dissipation is responsible of a pile-up of energy near the cutoff wave number k_c at the early transition. As a direct consequence of this pile-up, the dissipation is overestimated despite the nature of the numerical operator that is essentially sub-dissipative. At this coarse resolution, this erroneous dissipation eventually overdamps E_k for the rest of the calculation without being able to suppress the spurious energy at small scale. This behaviour is a very simple illustration of the contradictory conclusions that can be provided by *a priori* and *a posteriori* analysis of the influence of any subgrid-scale model.

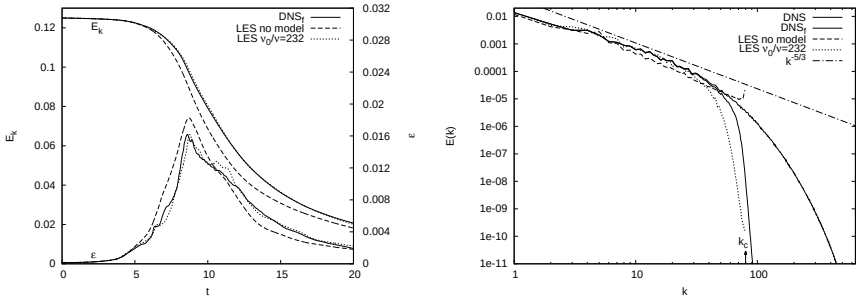

Fig. 3 Left: time evolution of the kinetic energy E_k and its dissipation ε. Right: 1D spectra $E(k,t)$ at $t = 24$.

Then, when the second derivatives of the Navier-Stokes equations are computed using an over-dissipative scheme with the level of numerical viscosity predicted by the Pao-like solver ("LES $\nu_0/\nu = 232$" case), the agreement with the filtered DNS is clearly improved as shown in figure 3 (left). The *a priori/a posteriori* paradox is recovered in reverse, namely the extra dissipation is found to slow down the time decrease of E_k by comparison with the "LES no model" case while matching

remarkably well the "DNS$_f$" data. This matching suggests that the artificial dissipation provided by the choice $\nu_0/\nu = 232$ is able to compensate consistently the small-scale dissipation that is missed by the coarse discretization.

To better understand the role played by the artificial viscosity, it is insightful to consider the time evolution of the kinetic energy spectrum $E(k,t)$. For the "LES no model", from the start of the early transition until the end of the calculation, an unrealistic pile-up of energy can be observed in the vicinity of the cutoff wave number k_c. This production of small-scale oscillations leads to very unrealistic vortical structures subjected to a spurious background noise in instantaneous visualisations of, for instance, the enstrophy and the Q-criterion (not shown for reasons of space). Conversely, the use of a calibrated numerical viscosity for the "LES $\nu_0/\nu = 232$" case enables a strong decrease of $E(k,t)$ at $k \approx k_c$ throughout the simulation. These behaviours are illustrated in figure 3 (right) for spectra obtained at $t = 14$, a time for which the turbulence is fully developed. The spectral range where the artificial dissipation is active can be easily guessed by comparison to the non-filtered DNS results. The resulting damping of the small-scale energy ensures the regularity of the LES solution (free from spurious oscillations) as for its numerically converged DNS counterpart computed at high resolution. This feature enables the development of realistic vortices that compare very well, at least qualitatively, to those associated with the filtered DNS results (not shown for reasons of space).

It can be noticed that the damping of the kinetic energy near k_c is stronger for the "LES $\nu_0/\nu = 232$" case compared to the "DNS$_f$" data. This discrepancy means that the Pao-like solver cannot predict exactly the full dissipation as it is actually computed in the LES. The assumption of turbulence in equilibrium to simplify the Lin equation can be suspected to be responsible of this inability. Another reason could be connected to the discretization errors in the convective terms that are not taken into account. The improvement of the present Pao-like model is in progress, in particular by taking into account the pervasive non-equilibrium nature of the turbulence. The potential benefit of non-vanishing spectral viscosity as in the subgrid-scale model of [1] is also under investigation.

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