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Assessing the numerical dissipation rate and viscosity in numerical simulations of fluid flows

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ABSTRACT

We propose a method for quantifying the *effective numerical dissipation rate* and *effective numerical viscosity* in Computational Fluid Dynamics (CFD) simulations. Different from previous approaches that were formulated in spectral space, the proposed method is developed in a physical-space representation and allows for determining numerical dissipation rates and viscosities locally, that is, at the individual cell level, or for arbitrary subdomains of the computational domain. The method is self-contained and uses only the results produced by the Navier–Stokes solver being investigated. As no further information is required, it is suitable for a straightforward quantification of numerical dissipation as a post-processing step. We demonstrate the method's capabilities on the example of implicit large-eddy simulations of a three-dimensional Taylor–Green vortex flow, serving as a test flow going through laminar, transitional, and turbulent stages of time evolution. For validation, we compare results for the effective numerical dissipation rate with exact reference data we obtained with an accurate, spectral-space approach.

1. Introduction

Results of numerical simulations of fluid flows are always contaminated by truncation errors introduced by the discretization of governing differential equations. Truncation errors are only negligible if all physical scales are well resolved by the given mesh and time-step size. For lower temporal or spatial resolution, however, truncation errors affect the simulation results and can be of similar magnitude as physical effects. This situation is most frequently encountered in numerical simulations of turbulent flows at high Reynolds numbers. Simulating such flows usually requires modeling contributions of unresolved scales by various turbulence modeling procedures, leading to Reynolds-averaged Navier–Stokes (RANS) simulations or large-eddy simulations (LES).

In recent years, it has been recognized that the truncation errors may even act as a substitute for modelling of non-resolved scales. In turbulence, this approach is known as monotonically integrated LES (MILES) or implicit LES (ILES), and was originally proposed by Boris et al. [1] and reviewed more recently in a monograph edited by Grinstein et al. [2]. With ILES, the Navier–Stokes equations are solved numerically on a coarse LES mesh without explicit SGS models. Often one relies on nonlinearly stable methods, such as total variation diminishing (TVD), flux-corrected-transport (FCT) and flux-limited and sign-preserving schemes [3–5], originally developed to control numerical oscillations in configurations involving steep gradients or discontinuities. In the stabilized spectral LES [6] the numerical stability is not provided by the truncation error of the numerical discretization (which is exponentially small for a spectral method [7]) but by the spectral filter that strongly attenuates the small resolved scales if applied at each time step. In the same spirit, Bogey and Bailly [8] use an explicit filter applied every few time steps as a substitute for a SGS model in LES of a turbulent jet flow. Such methodologies are justified on a basis of the practical observation that truncation errors in non-oscillatory methods, as well as explicit filtering, introduce numerical dissipation, and that they effectively act as SGS models. For instance, [9] report the development of the $k^{-5/3}$ inertial subrange in numerical simulations of isotropic turbulence performed using the piecewise parabolic method (PPM) implemented in an Euler solver. This is a nominally inviscid case where the kinetic energy should be conserved but in the simulations it decays in agreement with Navier–Stokes dynamics because of numerical dissipation. Despite a wealth of positive results it should be recognized that the presence of numerical dissipation or explicit filtering does not guarantee physically correct dynamics of the resolved scales. For example, Garnier et al. [10] analyzed several different

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shock-capturing Euler schemes applied to decaying isotropic turbulence and the conclusions were less favorable for ILES. While it was possible to obtain the inertial subrange, other results, such as probability densities of velocity derivatives and pressure, showed characteristics of low Reynolds number flows rather than what would have been expected from high Reynolds number LES. This behavior was attributed to the fact that the numerical dissipation often overwhelms the SGS dissipation computed for the same field using an explicit SGS model. Similar conclusions were drawn by Domaradzki and Radhakrishnan [11], who showed that the results obtained with the MPDATA method [12] for rotating and non-rotating turbulence were sensitive to the time-step size, and the method failed to produce theoretically expected results for certain initial conditions, and for rotating turbulence. The current rather vague definition of SGS modeling capabilities of the wide range of ILES schemes proposed in literature demands a more systematic approach to determine the effective dissipation aposteriori. Such a tool would allow comparisons of the effective numerical dissipation with the physical dissipation provided by resolved viscous stresses, and by explicit SGS models. Analytical information about the truncation errors can be obtained from the modified equation analysis but this approach is not feasible for multidimensional, nonlinear transport equations. The first aposteriori method for computing integral numerical dissipation has been proposed by Domaradzki et al. [13]. It is based on comparing flow evolutions from the same initial condition using two different discretization schemes, a scheme with finite numerical dissipation and a spectral code with negligible numerical dissipation. The method was used to analyze ILES simulations performed with the MPDATA approach for freely decaying high Reynolds number homogeneous turbulence with and without Coriolis forces Domaradzki and Radhakrishnan [11] and for a spectral multidomain simulations stabilized by spectral filtering and penalty methods Diamessis et al. [14]. The procedure computes the effective, wavenumber-dependent, numerical dissipation rate $\widehat{\mathcal{E}}_{n,sp}(\kappa,t)$ and the corresponding numerical viscosity $\hat{\nu}_{n,sp}(\kappa,t)$ for comparison with the analytical theories of turbulence. This procedure was employed by Hickel et al. [15] to develop a specific ILES method that is consistent with the physical energy transfer in turbulence, the so-called adaptive local deconvolution method (ALDM). It is based on a nonlinear discretization scheme which contains several free deconvolution parameters that allow to control its truncation error. The free parameters are constrained so that the numerical viscosity optimally matches the theoretical eddy viscosity predicted by the analytical theories of turbulence. While the optimization was performed for isotropic turbulence, the parameters of the scheme, once determined, proved to be valid also for simulations of other turbulent flows. Another method for estimating the numerical dissipation in LES was proposed recently by Zhou et al. [16] and is based on using the energy flux from the large, resolved scales as the numerical dissipation estimate.

The analysis of Domaradzki et al. [13] was developed in spectral space (to allow one-to-one comparisons with spectral eddy viscosities obtained from analytical theories of turbulence) and measures the global (spectral) dissipation rate. Despite being very accurate, Fourier-space based analysis of the numerical dissipation has some limitations. Since the computational domain must be periodic, the method cannot be easily generalized to non-periodic flows for which a local estimate of physical-space numerical dissipation is of particular practical interest. Also, using an additional spectral code for analysis is not always feasible.

The objective of this work is to develop and validate a more general procedure, free of the limitations listed above, for assessing the numerical dissipation rate for any given grid-based Navier–Stokes solver and a wide range of flows. The proposed method is equally applicable to periodic and non-periodic flows, provides a numerical-dissipation field, and can be employed as a post-processing tool for computational data.

2. Basic equations

The evolution of smooth and continuous fluid flows can be described by the conservation of mass, momentum and total energy. For a fluid with constant dynamic viscosity $\mu = \nu\rho$ as assumed for this study this set of equations, denoted as the Navier–Stokes equations (NSE), is

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_\alpha)}{\partial x_\alpha} = 0, \tag{1a}$$

$$\frac{\partial(\rho u_\alpha)}{\partial t} + \frac{\partial(\rho u_\alpha u_\beta)}{\partial x_\beta} = -\frac{\partial p}{\partial x_\alpha} + \mu \frac{\partial(\tau^{\alpha\beta})}{\partial x_\beta}, \tag{1b}$$

$$\frac{\partial(\rho e_t)}{\partial t} + \frac{\partial(\rho e_t u_\alpha)}{\partial x_\alpha} = -\frac{\partial(p u_\alpha)}{\partial x_\alpha} + \mu \frac{\partial(u_\beta \tau^{\alpha\beta})}{\partial x_\alpha} - \frac{\partial}{\partial x_\alpha}\left(k \frac{\partial T}{\partial x_\alpha}\right) \tag{1c}$$

The stress tensor is

$$\tau^{\alpha\beta} = \frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} - \frac{2}{3}\frac{\partial u_\gamma}{\partial x_\gamma}\delta_{\alpha\beta}, \tag{2}$$

u_α are the components of the velocity vector, p denotes the pressure, T is the temperature and k is the thermal conductivity. For when $\nu = 0$ the second term on the right-hand side of the momentum and total-energy transport equations, Eqs. (1b) and (1c), vanish and the system of conservation equations is denoted Euler equations. The transport of e_t can be separated into the transport equation for internal energy e_{in}

$$\frac{\partial(\rho e_{in})}{\partial t} + \frac{\partial(\rho e_{in} u_\alpha)}{\partial x_\alpha} = -p\frac{\partial(u_\alpha)}{\partial x_\alpha} + \mu\tau^{\alpha\beta}\frac{\partial(u_\beta)}{\partial x_\alpha} - \frac{\partial}{\partial x_\alpha}\left(k\frac{\partial T}{\partial x_\alpha}\right) \tag{3}$$

and kinetic energy $e_{kin} = \frac{1}{2}u_\alpha u_\alpha$

$$\frac{\partial(\rho e_{kin})}{\partial t} + \frac{\partial(\rho e_{kin} u_\alpha)}{\partial x_\alpha} = -u_\alpha\frac{\partial(p)}{\partial x_\alpha} + \mu u_\beta \frac{\partial(\tau^{\alpha\beta})}{\partial x_\alpha}. \tag{4}$$

The second term on the right hand side of Eq. (4) is the viscous contribution to the kinetic energy equation. To express the transfer of kinetic energy by viscous dissipation to the internal energy more clearly, the viscous contribution may be rewritten as

$$\mu u_\beta \frac{\partial(\tau^{\alpha\beta})}{\partial x_\alpha} = \mu\frac{\partial(u_\beta\tau^{\alpha\beta})}{\partial x_\alpha} - \mu\tau^{\alpha\beta}\frac{\partial(u_\beta)}{\partial x_\alpha}. \tag{5}$$

The first term on the right hand side of Eq. (5) is the the viscous work. Thus, the kinetic energy transport equation (for compressible flows) is:

$$\frac{\partial(\rho e_{kin})}{\partial t} + \frac{\partial(\rho e_{kin} u_\alpha)}{\partial x_\alpha} + u_\alpha\frac{\partial(p)}{\partial x_\alpha} - \mu\frac{\partial(u_\beta\tau^{\alpha\beta})}{\partial x_\alpha} + \mu\tau^{\alpha\beta}\frac{\partial(u_\beta)}{\partial x_\alpha} = 0. \tag{6}$$

Integration of the kinetic-energy transport Eq. (6) over the control volume $V = L_1 \times L_2 \times L_3$ leads to its integral form

$$\frac{\partial(E_{kin})}{\partial t} + F_{ekin} + F_{ac} - F_v - \Pi + \mathcal{E}_v = 0, \tag{7}$$

where

$$E_{kin} = \int_0^{L_1}\int_0^{L_2}\int_0^{L_3} \rho e_{kin} dx_1 dx_2 dx_3 \tag{8}$$

and the kinetic and acoustic energy fluxes as well as the viscous surface work are

$$F_{ekin} = \iiint_V \frac{\partial(\rho e_{kin} u_\alpha)}{\partial x_\alpha} dV = \iint_A n_\alpha(\rho e_{kin} u_\alpha) dA \tag{9}$$