Numerical dissipation and the bottleneck effect in simulations of compressible isotropic turbulence

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Abstract

Energy spectrum functions computed from data of various three-dimensional simulations of forced isotropic turbulence are investigated. The piece-wise parabolic method (PPM) was used to treat flows with Mach number of the order unity. The dissipation is of purely numerical origin. For the dimensionless mean rate of dissipation, we find values in agreement with results from other, mostly incompressible turbulence simulations. The so-called bottleneck phenomenon is also present in the turbulence energy spectra. Although the bottleneck reduces the range of nearly inertial scales considerably, we were able to estimate the value of the Kolmogorov constant. In the statistically stationary regime, \( C \approx 1.7 \) for strictly subsonic turbulence, but also in the presence of shocklets in moderately transonic flows. As compressive components become more significant, however, the value of \( C \) appears to decrease. Moreover, we discuss length scales related to numerical dissipation, in particular, an effective numerical length scale \( \Delta_{\text{eff}} \), which can be regarded as the characteristic smoothing length of the implicit filter associated with the PPM.

\textbf{Key words:} turbulence, turbulence modelling, compressible flows, dissipation, bottleneck effect, piece-wise parabolic method

\textbf{PACS:} 47.11.+j, 47.27.Eq, 47.27.Gs, 47.27.Gs, 47.40.Dc, 47.40.Hg, 97.60.Bw
1 Introduction

The paradigm of statistically stationary isotropic turbulence put forward by Kolmogorov is based on the balance between energy injection and dissipation in equilibrium, regardless of the detailed mechanism of dissipation. This implies the well-known scaling relation [1]

\[ E(k) = C\langle \epsilon \rangle^{2/3}k^{-5/3} \]  

for the turbulence energy spectrum in the inertial subrange. The universality of Kolmogorov scaling was confirmed in many laboratory experiments and three-dimensional numerical simulations [2,3,4,7,8,10,11,14]. For a certain equation of state, the mean rate of dissipation, \( \langle \epsilon \rangle \), is completely determined by the characteristic length and velocity scales, \( L \) and \( V \), respectively, of the flow. Normalising \( \langle \epsilon \rangle \) in terms of these scales, a dimensionless quantity is obtained:

\[ \langle \tilde{\epsilon} \rangle = \frac{L}{V^{3/2}}\langle \epsilon \rangle \]  

It is customary to specify the dimensionless rate of dissipation in terms of the similarity parameter \( C_\epsilon \sim \langle \tilde{\epsilon} \rangle \). The exact definition of \( C_\epsilon \) is given in section 4. Numerous attempts have been made to infer the value of \( C_\epsilon \) either from laboratory measurements in turbulent flows or numerical simulations. It appears that \( \langle \epsilon \rangle \) is generally of the order unity. Particularly, a universal value of about 0.5 for statistically stationary isotropic turbulence of sufficiently high Reynolds number has emerged over the last decade [11,12,13]. However, virtually all of the numerical estimates of \( C_\epsilon \) have been obtained from simulations of incompressible turbulence so far. Only very recently, first results from simulations of incompressible flows with higher-order finite difference methods have become available and, actually,  

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are in excellent agreement with previously reported values [16]. We will extend on this approach and present calculations of the instantaneous rate of dissipation from the energy budget in numerical simulations of forced compressible turbulence up to Mach numbers of the order unity. Moreover, the whole range of developing, steady and decaying turbulence is investigated. In order to make parameter studies feasible, we chose a rather moderate resolution of $432^3$.

The simulations we have performed also differ in other aspects from those cited above. Firstly, no explicit viscosity terms are included in the equations of motion. We use a high-order Godunov scheme, namely, the piece-wise parabolic method (PPM), which applies to fully compressible flows and, in fact, introduces *numerical dissipation* at a sufficiently high level to render additional Navier-Stokes viscous dissipation dispensable [5]. Of course, the question arises, whether the action of numerical dissipation mimics the effect of Navier-Stokes viscous dissipation properly [9,18]. We attempted to re-investigate this issue by means of turbulence energy spectra and parameters specifying the effect of numerical dissipation. In particular, we propose the definition of a characteristic length scale $\Delta_{\text{eff}}$ of the presumed implicit filter corresponding to the PPM. From the evaluation of simulation data, we found that the ratio $\beta = \Delta_{\text{eff}} / \Delta$ is about 1.6 for steady turbulence within the range of Mach numbers $\sim 0.1 \ldots 1$. This result is useful for the calibration of subgrid scale models for large-eddy simulations of turbulent deflagration, which actually motivated the work discussed in this article [19,20]. In particular, we are concerned with the modelling of thermonuclear deflagration in white dwarfs, which are thought to cause astronomical events known as type Ia supernovae [20,21]. For this reason, we used the equation of state of a degenerate electron gas in combination with non-degenerate nuclei in all of our turbulence simulations.

The spectra we computed from velocity field realisations of fully developed turbulence reveal a pile-up of kinetic energy near the wave number of maximum dissipation. This is known under the name *bottleneck effect* and was found in numerous numerical simulations [9,11,14]. The bottleneck is believed to be a genuine feature
of isotropic turbulence and can be attributed to the partial suppression of non-linear turbulent interactions under the influence of viscous dissipation [17]. Of course, the corresponding deviation from inertial scaling also bears consequences on the applicability of subgrid-scale models, in particular, those based upon similarity assumptions.

2 Forced isotropic turbulence

The dynamics of forced turbulence in compressible fluids is determined by the following set of conservation laws [22,23] in combination with the equation of state:

\[
\begin{align*}
\frac{\partial}{\partial t} \rho + \frac{\partial}{\partial x_i} \rho v_i &= 0, \\
\frac{\partial}{\partial t} \rho v_i + \frac{\partial}{\partial x_k} \rho v_i v_k &= -\frac{\partial}{\partial x_i} P + \rho f_i + \frac{\partial}{\partial x_k} \sigma_{ik}, \\
\frac{\partial}{\partial t} E + \frac{\partial}{\partial x_k} E v_k &= \rho f_k v_k.
\end{align*}
\]  

The field \( \vec{f}(\vec{x}, t) \) is called the driving force and may be any mechanical force acting upon the fluid and thereby supplying energy to the flow. The term \( \sigma_{ik,k} \) in the momentum equation accounts for the dissipation of kinetic energy. In the case of Navier-Stokes turbulence, the dissipation tensor \( \sigma_{ik} \) is proportional to the local strain of the velocity field:

\[
\sigma_{ik} = 2\rho \nu S^*_ik \equiv 2\rho \nu \left( S_{ik} - \frac{1}{3} v_{j,j} \delta_{ik} \right),
\]  

where \( S_{ik} = \frac{1}{2}(v_{i,k} + v_{k,i}) \). The coefficient \( \nu \) is the microscopic viscosity of the fluid.

According to the Landau criterion [22], the range of dynamically relevant length scales in a turbulent flow is of the order \( L/\eta_K \sim \text{Re}^{3/4} \), where \( L \) is the integral length scale associated with the spatial variation of the driving force, and \( \eta_K \), which
is called the *Kolmogorov scale*, is a characteristic length scale associated with viscous dissipation. If the Reynolds number \( \text{Re} = \frac{LV}{\nu} \) for a flow of characteristic velocity \( V \) is large enough, the range of dynamically relevant length scales will become computationally intractable. Then the common approach is to run a large-eddy simulation, which resolves only the largest scales and invokes some model for turbulence on smaller scales. On the other hand, it has been suggested to let merely the dissipative effect of finite-volume schemes smooth out the flow on length scales just above the numerical cutoff and dispose of accumulating kinetic energy [18].

The crucial hypothesis is that the flow statistics on scales \( l \gg \Delta \) is unaffected by the mechanism the characteristic length scale of dissipation. In particular, this assumption was put forward and exhaustively tested for the *piece-wise parabolic method* (PPM) [5,7,8,9].

We chose to follow the latter approach and adopted the PPM for simulations of forced isotropic turbulence. In order to produce fully developed turbulence, a random driving force was applied [24]. The evolution of the force field corresponds to a three-dimensional diffusion process in spectral space, with the Fourier transform \( \hat{\mathbf{f}}(\mathbf{k}, t) \) given by

\[
\frac{d}{dt} \hat{\mathbf{f}}(\mathbf{k}, t) = -\hat{\mathbf{f}}(\mathbf{k}, t) \frac{dT}{T} + F_0 \sum_{jlm} \left( \frac{2\sigma^2(\mathbf{k})}{T} \right)^{1/2} \delta(\mathbf{k} - \mathbf{k}_{jlm}) \mathbf P_{\mathbf{k}}(\mathbf{k}) \cdot d\mathbf{W}_t. \tag{7}
\]

The discretisation in physical space induces a discrete spectrum of modes associated with the wave vectors \( \mathbf{k}_{jlm} \). Gaussian random increments are introduced by the three-component *Wiener process* \( \mathbf{W}_t \) and are projected by means of the symmetric operator

\[
(\mathbf{P}_{ij})(\mathbf{k}) = \zeta \mathbf{P}_{ij}(\mathbf{k}) + (1 - \zeta) \mathbf{P}_{ij}^\perp(\mathbf{k}) = \zeta \delta_{ij} + (1 - 2\zeta) \frac{k_i k_j}{k^2}. \tag{8}
\]

For the spectral weight \( \zeta = 1 \), the physical force field becomes purely solenoidal, i.e., divergence-free. Choosing \( \zeta < 1 \), dilatational components are generated, which act to compress or rarify the fluid. The spectral profile of the driving force
is determined by the variance $\sigma^2(\vec{k})$. We use a symmetric quadratic function centred at the wave number $k_0$. For $k > 2k_0$, all modes of the force vanish identically. The integral length scale $L$ is defined by $L = 2\pi/k_0$. Once $\sigma(\vec{k})$ is normalised, the asymptotic RMS amplitude of the stochastic driving force depends on $F_0$ and the weight $\zeta$ only:

$$f_{\text{rms}} \simeq (1 - 2\zeta + 3\zeta^2)F_0.$$  \hspace{1cm} (9)

The simulations we have performed start with uniform fluid at rest. A grid of $432^3$ cells was used in each case for a domain of size $X = \alpha L$ with $\alpha = 3$. The magnitude of the driving force, $F_0$, was set equal to $V/T$, where $V$ is the characteristic velocity of the flow and $T$ the auto-correlation time of the driving force (see equation 7). Choosing $L$ and $V$ to be free parameters, the expectation that the time scale of the driving force determines the large-eddy turn-over time of the flow implies $T = L/V$. It was found that, depending on the Mach number and the spectral weight $\zeta$, a few large-eddy turn-overs elapse until turbulence has developed and the flow becomes statistically stationary. The parameters for several particular simulations are listed in table 1. Except for the lowest Mach number, transonic flows were produced, i.e., the fluid velocity exceeded the speed of sound in certain regions. As supplementary information, the duration $t_f$ of each simulation and the time $t_d$ at which the decay of turbulence started are listed. Given the astrophysical background of our work, we employed the equation of state of a degenerate electron gas [25]. This equation of state is encountered in so-called white dwarfs, which emanate from the burnout of stars comparable in mass to our Sun. Apart from the electrons, which constitute a so-called Fermi gas, there are non-degenerate nuclei. The nuclear component can be treated as an ordinary perfect gas, although it contributes only little to the total pressure.

The global statistics of a representative simulation is shown in figure. In this case, $V = 0.66c_0$ was chosen, where $c_0$ is the initial speed of sound. The spectral weight of forcing was set equal to $3/4$. Thus, the major component is solenoidal, but
there is a significant dilatational contribution as well. The plot of the RMS velocity
shown in the top left panel illustrates the different regimes in this simulation. In
the beginning, fluid is set into motion by the stochastic driving force. In the course
of production, the intensity of turbulence grows exponentially, as one can see from
the evolution of RMS vorticity in the bottom panel on the left. At \( t/T \approx 2.0 \),
the velocity flattens at a certain level corresponding to steady turbulence. At time
\( t/T = 5.0 \), the force field begins to decay exponentially and the energy contents of
the flow is subsequently dissipated. This is also illustrated by the time derivatives of
total, kinetic and internal energy, respectively, which are shown in the right bottom
panel of figure 3. Note that the specific energy gradually increases, because of the
continuous conversion of mechanical energy into heat by dissipation.

3 The energy spectrum function

The quintessence of isotropic turbulence is found in the spectrum of kinetic energy.
For developed turbulence at sufficiently high resolution, three subrange of wave
numbers can be distinguished. Firstly, the wave numbers of energy injection in the
vicinity of \( k_0 \), secondly, the inertial subrange in which the turbulence cascade reigns
and, finally, those wave numbers for which numerical dissipation dominates the dy-
namics. In this section, a discrete formulation of the turbulence energy spectrum is
devised. Since we are concerned with spatially periodic velocity fields, which are
not absolutely integrable, we shall first define the Fourier transform \( \hat{\vec{v}}(\vec{k}, t) \)
precisely. Assuming periodicity in \((x, y, z)\) with wavelengths \( X, Y \) and \( Z \), \( \hat{\vec{v}}(\vec{k}, t) \) can
be defined by a normalised volume integral,

\[
\hat{\vec{v}}(\vec{k}, t) = \int_{0}^{Z} \frac{dz}{Z} \int_{0}^{Y} \frac{dy}{Y} \int_{0}^{X} \frac{dx}{X} v(\vec{x}, t) \exp(-i\vec{k} \cdot \vec{x}).
\] (10)
The spatial region spanned by \((X, Y, Z)\) is the fundamental domain. The inverse Fourier transform consistent with the above definition of \(\hat{v}(\vec{k}, t)\) is given by

\[
\vec{v}(\vec{x}, t) = \frac{XYZ}{(2\pi)^3} \int d^3k \hat{v}(\vec{k}, t) \exp(i\vec{k} \cdot \vec{x}).
\] (11)

Periodicity in physical space induces a dual structure in spectral space in the form of an equipartition into cells of volume \((2\pi)^3/XYZ\). Each of these cells is associated with a wave vector \(\vec{k}_{jlm} = 2\pi(j/X, l/Y, m/Z)\). To that effect, any periodic function can be expressed as a discrete Fourier series, i.e.,

\[
\vec{v}(\vec{x}, t) = \sum_{j,l,m} \hat{v}_{jlm}(t) \exp(i\vec{k}_{jlm} \cdot \vec{x}),
\] (12)

where the Fourier modes are given by

\[
\hat{v}_{jlm}(t) = \int_0^\alpha d\tilde{z} \int_0^\alpha d\tilde{y} \int_0^\alpha d\tilde{x} \vec{v}(\vec{x}, t) \exp \left[ -\frac{2\pi i}{\alpha} (j\tilde{x} + l\tilde{y} + m\tilde{z}) \right],
\] (13)

with the dimensionless coordinates \(\tilde{x}_i = x_i/L \in [0, \alpha]\). Note that \(\hat{v}_{jlm}\) has the dimension of velocity. In order to consolidate the notion of a Fourier transform and the existence of discrete Fourier modes, \(\hat{v}(\vec{k}, t)\) has to be identified with the following generalised function:

\[
\hat{v}(\vec{k}, t) = \frac{(2\pi)^3}{XYZ} \sum_{jlm} \hat{v}_{jlm}(t) \delta(\vec{k} - \vec{k}_{jlm}).
\] (14)

Inspired by Parseval’s theorem, let us invoke the condition that the total kinetic energy integrated over all discrete Fourier modes must be equal to the mean kinetic energy in physical space:

\[
\langle e_{\text{kin}}(t) \rangle = \int_0^\alpha d\tilde{z} \int_0^\alpha d\tilde{y} \int_0^\alpha d\tilde{x} \frac{1}{2} \hat{v}(L\tilde{z}, t)^2 = \sum_{jlm} \frac{1}{2} \hat{v}_{jlm}(t) \cdot \hat{v}_{jlm}^*(t).
\] (15)
Obviously, this identity expresses the requirement of energy conservation. In the case of isotropic turbulence, the sum over all squared modes of the velocity field can be expressed as an integral over a function of the wave number only:

$$\int_0^\infty d(\alpha\tilde{k}) E(\alpha\tilde{k}, t) = \frac{1}{V^2} \sum_{jlm} \frac{1}{2} (\hat{v}_{jlm}(t) \cdot \hat{v}_{jlm}^*(t))$$  \hspace{1cm} (16)

Here the wave number is written in dimensionless form as $\tilde{k} = Lk/2\pi$. The function $E(k, t) = (\alpha L/2\pi)V^2\tilde{E}(\alpha\tilde{k}, t)$ is called the energy spectrum function. Expressing the right hand side of equation (16) as an integral,

$$\sum_{jlm} \frac{1}{2} (\hat{v}_{jlm}(t) \cdot \hat{v}_{jlm}^*(t)) = \int_0^\infty d(\alpha\tilde{k}) \sum_{jlm} \frac{1}{2} (\hat{v}_{jlm}(t) \cdot \hat{v}_{jlm}^*(t)) \delta[\alpha(\tilde{k} - \tilde{k}_{jlm})],$$  \hspace{1cm} (17)

where $\alpha\tilde{k}_{jlm} = (j^2 + l^2 + m^2)^{1/2}$, we obtain

$$\tilde{E}(\alpha\tilde{k}, t) = \frac{1}{V^2} \sum_{jlm} \frac{1}{2} (\hat{v}_{jlm}(t) \cdot \hat{v}_{jlm}^*(t)) \delta[\alpha\tilde{k} - (j^2 + l^2 + m^2)^{1/2}].$$  \hspace{1cm} (18)

In the above form, the energy spectrum function is still not suitable for numerical evaluation. Actually, a discrete counterpart of $\tilde{E}(\alpha\tilde{k}, t)$ is called for. To begin with, let us introduce a staggered mesh of wave numbers,

$$\mathcal{K} = \{0, k_{1/2}, k_1, k_{3/2}, \ldots \} = \{k_{(n-1)/2}|n \in \mathbb{N}\},$$

and define a discrete measure

$$\mu_n = \sum_{\alpha^2\tilde{k}_{n-1/2}^2 \leq \alpha^2\tilde{k}_n^2 \leq \alpha^2\tilde{k}_{n+1/2}^2} \sum_{jlm} \left(\frac{2\pi}{\alpha L}\right)^3 \delta^{\alpha^2\tilde{k}_n^2}_{j^2+l^2+m^2}$$  \hspace{1cm} (19)

associated with the wave number $k_n$. Note that the principal summation index $\alpha^2\tilde{k}_n^2 \in \mathbb{N}$. As one can see from the definition, $\mu_n$ is the total volume of all spectral cells of wavenumber $k_{jlm}$ within the interval $[k_{n-1/2}, k_{n+1/2}]$. The normalised measure $\bar{\mu}_n = (\alpha L/2\pi)^3 \mu_n$ is just the corresponding number of cells. The average
kinetic energy of modes with wave number \( k_{n-1/2} \leq k_{jlm} \leq k_{n+1/2} \) at time \( t \) is thus given by

$$
\Phi_n(t) = \frac{1}{\tilde{\mu}_n} \sum_{\alpha^2 k^2_{n-1/2} \leq \alpha^2 k^2 \leq \alpha^2 k^2_{n+1/2}} \sum_{jlm} \frac{1}{2} \tilde{v}_{jlm}(t) \cdot \tilde{v}_{jlm}^*(t) \delta_{j^2+i^2+m^2}.
$$

(20)

For small wave numbers \( \tilde{k}_n \sim 1 \), \( \Phi_n(t) \) clearly depends on the instantaneous state of the system. For large wave numbers \( \tilde{k}_n \gg 1 \), on the other hand, the above summation will cover a great number of cells, even if the interval \([\tilde{k}_{n-1/2}, \tilde{k}_{n+1/2}]\) is quite narrow, i.e., \( \tilde{k}_{n+1/2} - \tilde{k}_{n-1/2} \ll 1 \). Hence, in the case of statistically stationary isotropic turbulence, it can be expected that \( \Phi_n(t) \) approaches the ensemble average of \( \frac{1}{2} \tilde{v}_{jlm}(t) \cdot \tilde{v}_{jlm}^*(t) \) for large \( n \).

For this reason, we may conjecture that quasi-integration of \( \Phi_n(t) \) over the spherical shell of wave number \( k_n \) yields an approximation to the energy spectrum at least in the limit of large wave numbers. Defining

$$
\tilde{E}_n(t) = \frac{4\pi (\alpha \tilde{k}_n)^2}{V^2} \Phi_n(t),
$$

(21)

equation (20) implies

$$
\int_0^\infty d(\alpha \tilde{k}) \sum_n \tilde{E}_n(t) \frac{\tilde{\mu}_n}{4\pi (\alpha \tilde{k}_n)^2} \delta[\alpha(\tilde{k} - \tilde{k}_n)] = \frac{1}{V^2} \sum_{jlm} \frac{1}{2} (\tilde{v}_{jlm}(t) \cdot \tilde{v}_{jlm}^*(t)).
$$

(22)

By the meaning of this identity, we call \( \tilde{E}_n(t) \) the discrete energy spectrum function. On grounds of the ergodicity argument mentioned above, \( \sum_n \tilde{E}_n(t) \delta[\alpha(\tilde{k} - \tilde{k}_n)] \) can be regarded as approximation to the normalised energy spectrum function,

$$
\tilde{E}(\alpha \tilde{k}) = \frac{2\pi}{\alpha L} \cdot \frac{1}{V^2} E(k),
$$

(23)

where \( \tilde{\mu}_n d(\alpha \tilde{k})/4\pi (\alpha \tilde{k}_n)^2 \) is to be taken as the appropriate measure for the integration\(^1\). Averaging \( \tilde{E}_n(t) \) for steady turbulence over many integral time scales, the

\(^1\) In fact, the discrete and continuous points of view are reconciled by means of this mea-
approximation is expected to match the exact spectrum asymptotically.

The energy spectrum function can be separated into a longitudinal and a transversal part, in discrete form denoted by \( E_{\parallel n}(t) \) and \( E_{\perp n}(t) \), respectively. The longitudinal spectrum function is computed according to equations (20) and (21), with the Fourier modes \( \hat{v}_{jlm}(t) \) replaced by the modes projected parallel to the wave vector \( \vec{k}_{jlm} \),

\[
\hat{v}_{\parallel jlm} = \left( \frac{\vec{k}_{jlm} \cdot \hat{v}_{jlm}}{|\vec{k}_{jlm}|^2} \right) \vec{k}_{jlm}.
\]  

The transversal part of the spectrum function, on the other hand, is obtained by setting \( \hat{v}_{\parallel jlm}(t) = \hat{v}_{jlm}(t) - \hat{v}_{\parallel jlm}(t) \) in place of \( \hat{v}_{jlm}(t) \). Since

\[
|\hat{v}_{\parallel jlm}|^2 + |\hat{v}_{\perp jlm}|^2 = |\hat{v}_{jlm}|^2,
\]  

the sum of \( E_{\parallel n}(t) \) and \( E_{\perp n}(t) \) gives the total spectrum function \( E_n(t) \).

From the Kolmogorov spectrum function (1), it follows that \( \langle \epsilon \rangle^{-2/3} k^{5/3} E_{\perp}(k) \) is approximately constant in the inertial subrange of wave numbers. This suggests the definition of a compensated spectrum function,

\[
\Psi_{\perp n}(t) = \left[ \frac{\alpha}{2\pi} \langle \epsilon(t) \rangle \right]^{-2/3} \left( \alpha \tilde{k}_n \right)^{5/3} \tilde{E}_{\perp}(t),
\]  

as an indicator of Kolmogorov scaling. Note that only the transversal part of the energy spectrum is compensated, because it is the incompressible fraction of turbulence energy which \emph{a priori} fulfils Kolmogorov scaling. For the calculation of \( \Psi_{\perp n}(t) \), the mean dissipation rate \( \langle \epsilon \rangle \) has to be determined, and so we face the problem of numerical dissipation.

As an alternative, one might use \( d(\alpha \tilde{k}) \) as the right measure in both cases and renormalise the discrete energy spectrum function such that the correct integral is obtained. In that case, however, consistency would come at the cost of changing the energy in a certain wave number bin by a factor depending on the particular choice of the wave number grid \( K \) and the energy spectrum itself.
The rate of dissipation

The details of the numerical dissipation produced by the PPM are basically unknown, but it is possible to infer the net mean dissipation rate from the globally averaged energy conservation laws [23]. In fact, there are two distinct mechanisms of dissipation in a compressible fluid. On the one hand, pressure-dilatation accounts for the conversion of internal energy into mechanical energy and vice versa, as the fluid, respectively, expands or contracts. Although pressure-dilatation might locally produce mechanical work, it is effectively a dissipative, irreversible process, and the net rate of heat production is given by $-\langle Pd \rangle$. If pronounced shocks are present, however, there might be transient phases in which $\langle Pd \rangle$ becomes positive. Apart from the explicitly resolved pressure-dilatation, the dissipation is of numerical origin. Thus, we define the mean rate of dissipation $\rho_0 \epsilon_{\text{num}}$ from the averaged budget of internal energy. Since the boundary conditions are periodic, the total flux through the boundary surfaces cancels out, and we have

$$\rho_0 \epsilon_{\text{num}} = \frac{d}{dt} \langle E_{\text{int}} \rangle + \langle Pd \rangle. \quad (27)$$

The corresponding dimensionless rate of dissipation $\tilde{\epsilon}_{\text{num}}$ is defined by equation (2). Several representative values of $\tilde{\epsilon}_{\text{num}}$ and the ratio $-\langle Pd \rangle/\epsilon_{\text{num}}$ computed from DNS statistics are listed in the tables 2, 3 and 4.

In the literature it is common to normalise the rate of dissipation in terms of the RMS velocity fluctuation $v'$ and an integral length scale $\hat{L}$, which is defined by the transversal turbulence energy spectrum:

$$\hat{L} = \frac{\pi}{2v'^2} \int_0^{\pi/\Delta} \frac{E(k)^{\perp} \, dk}{k} \simeq \frac{L}{4v'^2} \sum_n \frac{\Phi_n^{\perp}}{k_n}. \quad (28)$$

The average kinetic energy $\Phi_n^{\perp}$ of transversal modes in the band $[k_{n-1/2}, k_{n+1/2}]$ is given by equation 20. For isotropic turbulence, $v'^2 = \frac{2}{3} \langle e_{\text{kin}} \rangle$, where $e_{\text{kin}} = \frac{1}{2} v^2$ is the specific kinetic energy. The parameter $C_\epsilon$ specifying the dimensionless rate of
dissipation is then given by
\[ C_\epsilon = \frac{\hat{L}}{\nu^{\frac{3}{2}}} \langle \epsilon_{\text{num}} \rangle. \] (29)

We attempted to estimate \( C_\epsilon \) from our simulation data as well. However, the results listed in tables 2, 3 and 4 must be considered with care. One reason is that we have not applied any time averaging, which smooths out variations of \( C_\epsilon \) due to different instantaneous realisations of the turbulent flow. Consequently, the listed values of \( C_\epsilon \) correspond to the instantaneous rate of dissipation and are subject to temporal variations. Another caveat is the calculation of \( \hat{L} \) from the discrete spectrum function \( E_n(k) \). Obviously, \( \hat{L} \) is mostly determined by the smallest wave numbers. Because only a few wave number bins are available for \( \tilde{k} \sim 1 \), errors in the numerical evaluation of the integral in equation (28) are inevitable.

The results for the parameter \( C_\epsilon \) corresponding to \( \bar{\epsilon}_{\text{num}} \) in the case of solenoidal stirring are listed in table 2. During the production phase, \( C_\epsilon \) is small compared to unity. Once equilibrium sets in, values of \( C_\epsilon \) in the range \( 0.4 \ldots 0.5 \) are found, which agree well with the time-averaged asymptote \( \bar{C}_\epsilon \approx 0.5 \) in simulations of incompressible turbulence [11,12,13]. In the decay regime, \( C_\epsilon \) increases gradually, which points towards enhanced viscous effects due to the diminishing inertial subrange. Comparing the values of \( C_\epsilon \) in table 2 with those listed in the tables 3, one can see that the behaviour is similar in both cases. As for the simulation with \( \zeta = 0.2 \), the values in table 4 appear to be more irregular, but not too different from the cases with dominating solenoidal components. Since there is no statistically stationary regime in the simulation with the highest Mach number, we cannot conclude what the corresponding asymptotic value of \( C_\epsilon \) might be. It is likely though that even in this case \( \bar{C}_\epsilon \approx 0.5 \) might hold for the transversal components of the velocity field.
5 Computed turbulence energy spectra

A number of spectra were computed from full data dumps at selected times. Some of these spectra are shown in Figures, and. For the calculation of the discrete spectrum function as given by definition (21), a coarse equidistant wave number mesh was used in the energy containing range, $0 \leq \tilde{k} \leq 2$, and a logarithmic mesh with narrow bins for the larger wave numbers. The panels on the top of figure show, from left to right, the discrete energy spectrum function $\tilde{E}_n(t)$ at representative stages in the production regime, the statistically stationary regime and, finally, in the advanced decay regime for the simulation with $\zeta = 1.0$ and characteristic Mach number $V/c_0 \approx 0.42$. For this simulation, a statistically stationary driving force was maintained for three integral times. At $\tilde{t} = 3.0$, the force field begins to decay. Also plotted are the longitudinal and transversal spectrum functions, $\tilde{E}_n^{\parallel}(t)$ and $\tilde{E}_n^{\perp}(t)$, respectively. In the bottom panels of figure, one can see the corresponding compensated spectrum functions $\tilde{\Psi}_n^{\perp}(t)$, which are defined by equation (26). In particular, the graph of $\tilde{\Psi}_n^{\perp}(t)$ for $t = 3.0$ verifies the existence of a narrow window of wave numbers in the vicinity of $\tilde{k} = 3.0$, in which Kolmogorov scaling with $C \approx 1.7$ applies approximatively. For the non-equilibrium stages at $t/T = 1.5$ and $t/T = 6.0$, on the other hand, we observe a different magnitude of the compensated spectrum function in this wave number region. At early time, dissipation is small and, consequently, the values of $\tilde{\Psi}_n^{\perp}(t)$ are larger for a given wave number. In the decay regime, the energy contents of the lower wave numbers diminishes rapidly and the corresponding portion of the energy spectrum is eroded. It is noteworthy that the value we found for $C$ in the stationary regime is very close to results obtained from other numerical simulations, especially, those with higher resolution [4,10,11]. However, the Kolmogorov constant inferred from our simulations might be systematically too large, because of the lack of isotropy for wave numbers close to the energy-containing subrange [4]. Moreover, the recently found indications for a modification of the Kolmogorov exponent by $-0.1$ [11] are consistent with our spectra in the vicinity of $\tilde{k} \approx 3$, although the lack of a sufficiently extended inertial
subrange does not allow us to draw any definite conclusions.

More or less the same behaviour is found in the case of the simulation with higher characterisic Mach number, \( V/c_0 \approx 0.66 \), and \( \zeta = 0.75 \). The sample spectra shown in figure are very similar in shape compared to those in figure , except for the smaller gap between the total and the longitudinal energy spectrum functions. Once more, the compensated spectrum function around \( \tilde{k} = 3.0 \) implies \( C \approx 1.7 \) at time \( \tilde{t} = 5.0 \), when the partially dilatational driving force begins to decay. As for the case \( \zeta = 0.2 \) and \( V/c_0 \approx 1.39 \), differences can evidently be seen in figure . Obviously, there is a significant fraction of turbulence energy in the longitudinal components of the Fourier modes. At early time, the flow is dominated by large-scale shock waves and most of the energy is contained in longitudinal modes. This is illustrated by the plot of the energy spectrum functions at time \( \tilde{t} = 2.0 \). The scaling deviates markedly from the Kolmogorov law. In particular, the longitudinal component \( E_n^\parallel(t) \) clearly obeys a power law with exponent \(-2\) and the transversal component is falling off even steeper. From the analysis of the simulation statistics, a transition to the shocklet-regime at time \( \tilde{t} \approx 3.0 \) can be discerned [6]. In this regime, the small-scale dynamics is eventually dominated by the turbulent vortex cascade as in the case of subsonic turbulence, and the transversal component of the energy spectrum function is more or less Kolmogorovian. However, we have a somewhat smaller value of the Kolmogorov constant, \( C \approx 1.3 \), at time \( \tilde{t} = 5.0 \) (see the middle panels in figure ). Therefore, it appears that the universality of the Kolmogorov law faces its limitations once a large proportion of the flow becomes supersonic and significant non-rotational components of the velocity field are produced.

For steady or decaying turbulence, there is a pronounced maximum of the compensated spectrum function at \( \tilde{k} \approx 15 \) corresponding to a flattening of the energy spectrum in comparison to the Kolmogorov law. This so-called bottleneck effect has actually been observed in various numerical simulations [3,9,14,15]. In the production phase, on the other hand, the spectrum does not exhibit a bottleneck. This is reasonable, because at the beginning the turbulence cascade is still building up and
the small-scale features, which cause the distortion of the spectrum seen at later time, are yet not fully developed. The anomalous bottleneck scaling is attributed to dynamical peculiarities on scales which are significantly influenced by dissipation. For example, experimental data indicate a $k^{-1}$ power law behaviour of the energy spectrum function in the vicinity of the wave number of maximum dissipation [2]. A theoretical explanation of the bottleneck effect on grounds of the non-linear turbulent transfer was suggested too [17]. In any case, the peaks of $\tilde{\Psi}_n(t)$ close to the wave number $\tilde{k} \approx 15$ are quite distinct, and there is certainly a significant pile-up of energy in modes of wave numbers $\tilde{k} \gtrsim 10$, once turbulence is fully developed. This might be caused at least in part by differences between the numerical dissipation produced by the PPM and viscous dissipation of physical origin (or the action of SGS stresses). The dependence of the bottleneck effect on the details of dissipation has recently been investigated for turbulence with hyper-viscosity [15]. Although the viscosity clearly influences the height of the bottleneck, the spectral width appears to be invariant.

6 Dissipation length scales

One can regard the action of numerical dissipation as being equivalent to an implicit filter smoothing the flow on a certain length scale, say, $\Delta_{\text{eff}}$. Fourier modes of wave number larger than $\pi/\Delta_{\text{eff}}$ are suppressed by the filter. The corresponding dimensionless cutoff wave number is $\tilde{k}_c = N/2\alpha = 72$. The ratio $\beta = \Delta_{\text{eff}}/\Delta$ is of particular interest for subgrid scale models based upon dynamical procedures, which depend on the reliable specification of the characteristic length scale associated with the finite-volume method [26,27]. It is customary, to set this length scale equal to the grid resolution $\Delta$, assuming a sharp cutoff associated with the numerical discretisation. If the PPM is used, however, this is not an appropriate choice. Although the common point of view holds that it is not sensible to apply a subgrid scale model in combination with highly dissipative schemes such as the PPM, in-
formation about subgrid scale turbulence is passively turned to account in certain applications. Especially, for the problem of turbulent burning, an effective flame propagation speed is computed from the local value of subgrid scale kinetic energy [19,20].

An improved estimate of the effective length scale $\Delta_{\text{eff}}$, which accounts for the dissipation produced by the PPM, makes use of the notion of a characteristic filter scale [28]. For a one-dimensional filter of explicitly known functional form, a characteristic length scale can be calculated from the second moment of the Fourier transform of the filter kernel, the so-called transfer function. Since the implicit filter associated with the PPM is not explicitly known, we have to resort to the numerically computed energy spectra. Using Kolmogorov’s law as reference spectrum function, let us introduce an effective transfer function

$$\hat{G}_{\text{eff}}^2(k, t) = \frac{E(k, t)}{E_{\infty}(k, t)} = \frac{1}{C} \Psi(k, t),$$

(30)

where $E_{\infty}(k, t) = C\epsilon_{\text{num}}^{2/3}(t)k^{-5/3}$. The second moment of the squared transfer function is defined by

$$M^{(2)}[\hat{G}_{\text{eff}}^2] = \int_0^\infty k^2 \hat{G}_{\text{eff}}^2(k, t)dk.$$  

(31)

Of course, the numerically computed spectrum function $E(k, t)$ is not conform with the Kolmogorov law at wave numbers comparable to $k_0 = 2\pi/L$, because of energy injection on the largest length scales. However, the contribution of these wave numbers to the above integral is small due to the factor $k^2$. Thus, we will ignore this error. Discretising the transfer function in the fashion outlined in section 3 and cutting off at the wavelength $\pi/\Delta$, the following approximation to the second moment

---

2 Usually, filter length scales are defined by the second moment of $\hat{G}$ rather than $\hat{G}^2$. Computationally, however, it is preferable to use the square of the transfer function.
is obtained:

\[
M^{(2)}[\hat{G}^2_{\text{eff}}] \simeq \frac{1}{C} \left( \frac{2\pi}{\alpha L} \right)^3 \int_0^{N/2} d(\alpha \tilde{k}) \sum_n \Psi_n(t) \frac{\tilde{\mu}_n}{4\pi} [\alpha(\tilde{k} - \tilde{k}_n)].
\]  

(32)

The second moment of the filter transfer function has the dimension of inverse length cubed. Hence, a length scale is given by \( (M^{(2)}[\hat{G}^2])^{-1/3} \) and customarily normalised with respect to the second moment of the sharp cutoff filter. The transfer function of this filter is given by \( \hat{G}_\Delta(k) = \theta(\pi/\Delta - k) \), and the second moment is \( M^{(2)}[\hat{G}^2_\Delta] = (\pi/\Delta)^3/3 \). Setting \( M^{(2)}[\hat{G}^2_{\text{eff}}] = (\pi/\Delta_{\text{eff}})^3/3 \), the effective filter scaling factor of the PPM is therefore estimated to be

\[
\beta = \frac{\Delta_{\text{eff}}}{\Delta} = \frac{N}{2} \left[ \frac{3}{C} \sum_{n=1}^{n_c} \Psi_n(t) \frac{\tilde{\mu}_n}{4\pi} \right]^{-1/3},
\]  

(33)

where \( n_c = \max\{n|\tilde{k}_n \leq \tilde{k}_c\} \). Several values of \( \beta \) determined from simulation data are listed in the tables 2, 3 and 4. The results demonstrate that \( \Delta_{\text{eff}} \approx 1.6\Delta \) is the more or less universal relation for fully developed turbulence. However, from yet another simulation with solenoidal stirring and \( V/c_0 \approx 0.084 \), the scaling factor \( \beta \approx 1.8 \) was found in the stationary regime. Consequently, the effect of numerical dissipation appears to become more pronounced for decreasing Mach number. This might be an indication of the PPM being not really suitable for low Mach number flows. Of course, the dependence of \( \beta \) on the numerical resolution should be investigated too. Changes can be expected towards lower resolution, because the energy-containing and the dissipation subrange will increasingly overlap. At higher resolution, on the other hand, \( \beta \) should asymptotically approach a value independent of \( N \). Unfortunately, the attempt to validate this conjecture would have required an undue amount of computational resources.

In fact, \( \Delta_{\text{eff}} \) is much smaller than the length scale of maximum dissipation, \( l_p \), which is given by the maximum of \( \tilde{k}_n^2 \tilde{E}_n(t) \propto \tilde{k}_n^{1/3} \tilde{\Psi}_n(t) \). For fully developed turbulence, the peak of dissipation was found to be located close to the second
maximum of $\tilde{\Psi}_n(t)$, with a typical value $l_p \approx 0.065L$ (see tables 2, 3 and 4). Note that $l_p$ is by about a decade smaller than the typical length scales, for which the Kolmogorov constant was estimated. Due to the bottleneck effect, however, even these scales are at least marginally affected by non-inertial range scaling. The flow structure on scales $l \gtrsim l_p$ can be extracted by explicitly smoothing the velocity field with a filter of sufficient characteristic length. In particular, a Gaussian filter of characteristic length scale $\Delta_G = 2l_p$ was applied to the spectral representation of velocity data from one of the simulations. The transfer function of the Gaussian filter is [29]

$$\hat{G}_G(\alpha \tilde{k}) = \exp \left[ -\frac{\pi^2}{6} \left( \frac{\Delta_G}{\alpha L} \right)^2 (\alpha \tilde{k})^2 \right]. \quad (34)$$

The filtered Fourier modes are then given by $\langle \hat{\vec{v}}_{jlm} \rangle_G = \hat{G}_G(\alpha \tilde{k}_{jlm}) \hat{\vec{v}}_{jlm}$, and the corresponding velocity field $\langle \vec{v} \rangle_G(\vec{x}, t)$ is obtained by computing the inverse Fourier transform. Basically, the filter operation removes the more random velocity fluctuations on the smallest scales, while vortical structures in the inertial subrange are preserved. This is illustrated in Figure , which shows a planar section through the filtered velocity field together with contours of the fully resolved velocity $v = (v_i v_i)^{1/2}$ in the case of purely solenoidal forcing at the end of the stationary regime ($\tilde{t}_d = 3.0$).

7 Conclusion

The computation of turbulence energy spectrum functions reveals several important properties of turbulence in numerical simulations with the PPM: Firstly, the range of length scales approximately satisfying Kolmogorov scaling, secondly, characteristic scales associated with numerical dissipation, and thirdly, the so-called bottleneck effect, i.e., an excess of kinetic energy in modes affected by dissipation.

In particular, it was shown that for the simulations of forced isotropic turbulence discussed in this paper, there is only a marginal inertial subrange. Nevertheless,
we were able to estimate the Kolmogorov constant for samples of the flow in quasi-equilibrium to be $C \approx 1.7$, which agrees very well with published results from more elaborate simulations. Moreover, this value was also verified for the solenoidal fraction of turbulence energy in moderately transonic flows, although indications of a reduction of the Kolmogorov constant were found in the case of a simulation with Mach number of order unity and forcing dominated by dilatational components. The parameter $C'_e$ specifying the dimensionless rate of numerical dissipation assumes values of about 0.5 for steady turbulence. This is consistent with the time-averaged asymptotic value in the limit of large Reynolds numbers calculated from simulations of incompressible turbulence. On the basis of the notion of an implicit filter, we define the length scale $\Delta_{\text{eff}}$ specifying the characteristic length of smoothing due to the numerical scheme. The ratio $\beta = \Delta_{\text{eff}}/\Delta$ appears to be fairly universal for statistically stationary turbulence. In the case of the PPM, $\beta \approx 1.6$. Furthermore, it was demonstrated that the computed spectra exhibit a pronounced bottleneck effect. The corresponding peak in the compensated spectrum functions closely coincides with the wave number of maximum dissipation.

In essence, the presented results suggest that numerical simulations of turbulence using the piece-wise parabolic method are indeed sensible and in good agreement with other methods based upon spectral computation of incompressible flows and explicit treatment of viscous dissipation.

8 Acknowledgements

The turbulence simulations were run on the Hitachi SR-8000 supercomputer of the Leibniz Computing Centre in Munich, using 512 processors in parallel, and the post-processing of the data was performed on a shared-memory node of the IBM p690 supercomputer of the Computing Centre of the Max-Planck-Society in Garching, Germany. We thank M. Reinecke, who was very helpful with technical advice. For the post-processing of the data, in particular, the Gaussian filtering, the FFTW
implementation of the the fast Fourier transform algorithm was utilised [30]. One of the authors (W. Schmidt) was supported by the priority research program Analysis and Numerics for Conservation Laws of the Deutsche Forschungsgesellschaft.

References


List of Figures

Fig. 1. Evolution of dimensionless mean quantities for a simulation forced isotropic turbulence in three dimensions. The characteristic Mach number is $V/c_0 = 0.42$ and the spectral weight of the driving force $\zeta = 0.75$. The panels show the RMS momentum and specific force, the mean total and internal energy, the RMS vorticity and divergence as well as the averaged rates of energy production and dissipation as functions of the normalised time $\tilde{t} = t/T$.

Fig. 2. Turbulence energy spectra for $V/c_0 = 0.42$ and $\zeta = 1.0$. The panels in the row on the top show the instantaneous discrete energy spectrum functions at representative stages in the advanced production regime, near equilibrium and in the late decay regime. In the bottom panels, the corresponding compensated spectrum functions are plotted.
Fig. 3. Turbulence energy spectra for $V/c_0 = 0.66$ and $\zeta = 0.75$.

Fig. 4. Turbulence energy spectra for $V/c_0 = 1.39$ and $\zeta = 0.2$.

Fig. 5. Flow map of the projected filtered velocity field $(\langle v_x \rangle_G, \langle v_y \rangle_G, 0)$ with contours of the fully resolved magnitude of the velocity, $\tilde{v} = (v_x^2 + v_y^2 + v_z^2)^{1/2}$, for the DNS with $\zeta = 1.0$ and $V/c_0 = 0.42$. The applied filter is Gaussian, with twice the length scale of maximum dissipation chosen as characteristic filter width. The arrows depicting the filtered velocity are normalised such that a length equal to the spacing $6\Delta/L$ between contiguous arrows corresponds to a magnitude $(\langle v_x \rangle_G^2 + \langle v_y \rangle_G^2)^{1/2} = V$. 

Table 1

Chosen values of the spectral weight $\zeta$ of the driving force, the characteristic Mach number $V/c_0$, the onset of decay $t_d/T$ and the end of each simulation $t_f/T$, as well as the total number of time steps $N_{\Delta t}$.

<table>
<thead>
<tr>
<th>$\zeta$</th>
<th>$V/c_0$</th>
<th>$t_d/T$</th>
<th>$t_f/T$</th>
<th>$N_{\Delta t}$</th>
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<td>$\bar{\epsilon}_{\text{num}}$</td>
<td>$-\langle Pd \rangle / \rho_0 \epsilon_{\text{num}}$</td>
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Table 2
Mean energy, rate of dissipation and characteristic length scales for a DNS with $V/c_0 = 0.42$ and $\zeta = 1.0$.

<table>
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<th>$\ddot{t}$</th>
<th>$\langle \tilde{e}_{\text{kin}} \rangle$</th>
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<th>$\bar{\epsilon}_{\text{num}}$</th>
<th>$-\langle Pd \rangle / \rho_0 \epsilon_{\text{num}}$</th>
<th>$C_\epsilon$</th>
<th>$\bar{L}/L$</th>
<th>$l_p/L$</th>
<th>$\beta$</th>
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Table 3
Mean energy, rate of dissipation and characteristic length scales for a DNS with $V/c_0 = 0.66$ and $\zeta = 0.75$.

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<th>$\bar{\epsilon}_{\text{num}}$</th>
<th>$-\langle Pd \rangle / \rho_0 \epsilon_{\text{num}}$</th>
<th>$C_\epsilon$</th>
<th>$\bar{L}/L$</th>
<th>$l_p/L$</th>
<th>$\beta$</th>
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<td>1.68</td>
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Table 4
Mean energy, rate of dissipation and characteristic length scales for a DNS with $V/c_0 = 1.39$ and $\zeta = 0.2$. 

Fig. 1
Fig. 2
Fig. 3
Fig. 4