Gas Kinetic Scheme for DNS of Decaying Compressible Turbulence

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We apply the gas-kinetic scheme (GKS) for direct numerical simulation (DNS) of compressible decaying homogeneous isotropic turbulence. We compute dynamics of the kinetic energy $K(t)$, the dissipation rate $\varepsilon(t)$, the probability density functions (PDFs) of the two-point longitudinal velocity difference $\delta u(\delta r)$ with a separation distance $\delta r$, the shocklet strength $\chi$, and the local Mach number $Ma$. Our results show that, (a) With initial Taylor microscale Reynolds number $Re_\lambda$ fixed, the maximum dissipation rate $\varepsilon$ attained at the initial stage increases as the initial turbulent Mach number $Ma_t$ increases; (b) The initial turbulence Mach number $Ma_t$ has no observable effect on kinetic energy $K(t)$ and the asymptotic behavior of the dissipation rate $\varepsilon(t)$; (c) At the lower $Ma_t (=0.1)$, the PDF of $\delta u(\delta r)$ for some $\delta r$ remain non-Gaussian for a long time, indicating persisting intermittency, while at higher $Ma_t (= 0.5)$, the PDF of $\delta u(\delta r)$ quickly becomes Gaussian regardless $\delta r$. And (d) The PDF's of both shock strength and the local Mach number all obey a scaling law.

I. Introduction

Technical feasibility of hypersonic flight, to an important degree, depends on our ability to understand and predict transition and turbulence in hypersonic flows with non-equilibrium thermo-chemistry.1, 2 In non-thermochemical-equilibrium (NTE) turbulence, however, the Kolmogorov paradigm, which forms the basis of most equilibrium turbulence models, is questionable. This is due to the fact that there can be baroclinic-type production of energy at all scales of turbulence, including the inertial range, invalidating the Kolmogorov hypotheses. Consequently, the premises of large-eddy simulations and other popular closures are not completely valid, and thus the turbulent mass, energy and momentum transport in NTE turbulence may not be amenable to standard treatment. Hence, physics-based modeling of NTE turbulence must start from fundamental first principles. At the same time, the simulation of highly NTE-turbulent flows is a challenge to the conventional computational fluid dynamics (CFD) based on the Navier-Stokes equation, because, under extreme conditions (high Mach and Reynolds numbers, moderate Knudsen number, high temperature and thermochemical nonequilibrium), the assumption of linear constitutive laws and even the basic premises of continuum mechanics begin to break down. As a result, the kinetic methods, which are derived from the Boltzmann equation as opposed to conventional CFD methods based on direct discretizations of the Navier-Stokes equations, have been attracting more and more attention in the recent years.

In contrast with the conventional CFD method, kinetic methods have two distinctive features. First, kinetic methods can include extended hydrodynamics beyond the validity regime of the Navier-Stokes equations, because they are based on kinetic theory. It is known that the Boltzmann equation provides the theoretical connection between hydrodynamics and the underlying microscopic physics. Kinetic methods are often called mesoscopic methods for they act between the macroscopic conservation laws and their corresponding microscopic dynamics. And second, the Boltzmann equation is a first-order integro-partial-differential equation with a linear advection term, while the Navier-Stokes equation is a second-order partial differential equation with a nonlinear advection term. The nonlinearity in the Boltzmann equation resides...
in its collision term, which is local. This feature may lead to some computational advantages. For these two reasons, kinetic methods have attracted more interest recently. Due to their mesoscopic nature, kinetic methods are particularly appealing in modeling and simulations of complex fluids.

There are a number of kinetic or mesoscopic methods, such as the lattice gas cellular automata (LGCA), the lattice Boltzmann equation (LBE), the gas-kinetic schemes (GKS), the smoothed particle hydrodynamics (SPH), and the dissipative particle dynamics (DPD). Among these methods, the LBE and GKS methods are specifically designed to as numerical methods for CFD: the former is for low-Mach-number flows while the latter is for fully compressible flows. Both methods have found extensive applications in many areas of flow physics. Some studies on direct numerical simulations (DNS) of turbulence have also been performed using kinetic methods, of which Lattice Boltzmann Equation (LBE) method was applied to the three-dimensional (3D) incompressible decaying homogeneous isotropic turbulence (DHIT). The DHIT is an important benchmark problem in the field of DNS of turbulence. The simulation of DHIT is sensitive to numerical dissipations in small scales. The LBE method has proved to be a highly reliable DNS tool for incompressible turbulence.

The final goal of our work is to develop a physics-based multiscale GKS for direct numerical simulations and large eddy simulations (LES) of nonequilibrium turbulent gas flows. In our previous work, we have applied both LBE and GKS to compute DHIT at a very low Mach number and performed detailed comparisons for those two kinetic methods at the incompressible limit. In the current paper, we are conducting the DNS of compressible DHIT using the GKS. In compressible DHIT, the gas compressibility admits the production of random shocklets, which is not observed in incompressible decaying turbulence. Blaisdell et al. performed pseudo-spectral simulations for compressible DHIT with the initial root-mean-square Mach number 0.05–0.7 and the initial Taylor microscale Reynolds number $\text{Re}_\tau$ at $O(50)$. Lee et al. used a sixth-order compact finite difference scheme to obtain results from $64^3$ and $128^3$ simulations with their largest $\text{Re}_\tau = 50$ and largest turbulent Mach number $M_a = 0.612$. Erlebacher et al. performed a DNS for DHIT with a split numerical method and a Fourier collocation pseudospectral method to evaluate the spatial derivatives on $64^3$, $96^3$, and $128^3$ grids. Kida and Orszag used a pseudospectral collocation method to carry out the simulations of compressible DHIT. In their simulations they detected and studied curved shocks. Samtaney et al. derived a model for the probability density function (PDF) of the shocklet strength based on weak shock theory and PDF of velocity differences. Based on the work of Samtaney et al., we apply the GKS for DNS of the compressible DHIT to obtain the detailed results and statistics on grids $128^3$ and $256^3$. Our numerical results show that the PDFs of both shock strength $\chi$ and the local Mach number $M_a$ obey a scaling law.

The remaining part of this paper is organized as follows. We provide the formulations of the GKS methods in Section II. We report the numerical results of compressible DHIT using GKS methods in Section III. We present the time evolution of kinetic energy, dissipation rate and the PDF’s of the two-point longitudinal velocity difference and the shocklet strength obtained by the GKS method. We conclude the paper in Section IV.

II. Numerical Methods

A. Description of Gas Kinetic Scheme

We shall describe the construction of the gas-kinetic scheme (GKS) for compressible flows. We begin with the linearized Boltzmann equation:

$$\partial_t f + \xi \cdot \nabla f = \mathcal{L}(f, f),$$

where $f := f(\mathbf{x}, \xi, \zeta, t)$ is the single particle distribution function of space $\mathbf{x}$, particle velocity $\xi$, particle internal degree of freedom $\zeta$ of dimension $Z$, and time $t$; $\mathcal{L}$ is the linearized collision operator. For the sake of simplicity, and without losing generality in the context of the linearized Boltzmann equation, we will use the Bhatnagar-Gross-Krook (BGK) single relaxation time model for $\mathcal{L}$:

$$\partial_t f + \xi \cdot \nabla f = -\frac{1}{\tau} \left[ f - f^{(0)} \right].$$

Here $\tau$ is the collision time and $f^{(0)}$ is the Maxwellian equilibrium distribution function in $D$ dimensions,

$$f^{(0)} = \rho \left( \frac{\beta}{2\pi} \right)^{(D+Z)/2} e^{-\beta(\mathbf{e} \cdot \mathbf{e} + \zeta^2)},$$

where $\rho$ is the internal degree of freedom, and $\beta = 1/\kappa T$ is the inverse temperature.
Thus, \( x \) position is the peculiar velocity, \( \beta = (RT)^{-1} \), \( R \) is the gas constant, and \( \rho, \mathbf{u} \) and \( T \) are the density, flow velocity and temperature, respectively.

By integrating along the characteristics, one can obtain the following solution of the BGK equation (2),

\[
f(x + \xi t, t) = e^{-t/\tau} f_0 + \frac{1}{\tau} \int_0^t f^{(0)}(x', \xi, \zeta, t') e^{(t-t')/\tau} dt',
\]

where \( x' := x + \xi t' \), and the initial state \( f_0 := f(x, \xi, \zeta, t = 0) \). The gas-kinetic scheme (GKS) is formulated based on the above equation. With \( f_0 \) and \( f^{(0)} := f^{(0)}(x, \xi, \zeta) \) given, one can construct an approximate solution for \( f \) at a later time \( t > 0 \).

The gas-kinetic scheme is a finite volume method for compressible flows. Thus, the values of the conserved variables are given at cell centers, while the values of fluxes are needed at cell boundaries. Unlike conventional CFD methods which evaluate fluxes from the hydrodynamic variables, the gas-kinetic scheme computes the numerical fluxes from the distribution function \( f \). In this study, we focus on the three-dimensional (3D) flows in which the total number of internal degrees of freedom is \( Z = (5 - 3\gamma)/(\gamma - 1) \) and \( \gamma = c_p/c_v \) is the ratio of specific heats.

For the sake of convenience, we shall use the following notation for the vectors of \((D + 2)\) dimensions,

\[
\mathbf{\Psi} := (1, \xi, (\xi^2 + \zeta^2)/2)^T, \quad (5a)
\]

\[
\mathbf{W} := (\rho, \rho \mathbf{u}, \rho E)^T = \int f \mathbf{\Psi} d\mathbf{\Xi} = \int f^{(0)} \mathbf{\Psi} d\mathbf{\Xi}, \quad (5b)
\]

\[
\mathbf{F}_\alpha := \int f \xi_\alpha d\mathbf{\Xi}, \quad \alpha \in \{x, y, z\} := \{1, 2, 3\}, \quad (5c)
\]

\[
\mathbf{h} := (\rho, \mathbf{u}, T)^T, \quad (5d)
\]

\[
\mathbf{h}' := (\rho^{-1}, \beta \mathbf{u}, 1/2 [\beta (\xi^2 + \zeta^2) - (D + Z) T^{-1}])^T, \quad (5e)
\]

where \( \mathbf{T} \) denotes the transpose operator. In the above notation, \( \mathbf{\Psi}, \mathbf{W}, \mathbf{F}_\alpha \) and \( \mathbf{h} \) have the collisional invariants, the conserved quantities, the fluxes along the \( \alpha \)-axis and the primitive variables as their components, respectively. According to Eq.(5b), the conserved variables are the conserved moments of the collision operator. \( E \) is the specific total energy with \( \rho E = \rho \epsilon + \frac{1}{2} \rho u^2 \) where \( \epsilon := \frac{1}{2} (D + Z) k_b T \) is the specific internal energy and \( k_b \) is the Boltzmann constant. \( \mathbf{\Xi} := (\xi, \zeta) \) denotes the single particle velocity space and the internal degrees of freedom. The Maxwellian equilibrium leads to the equipartition of energy among the degrees of freedom, i.e., each degree of freedom shares the same amount of energy \( k_b T/2 \) at equilibrium.

Here we are going to construct a multidimensional gas kinetic scheme in three dimensions, where the gradients of flow variables in both normal and two tangential directions around a cell interface are considered in the flux evaluation. To simplify the ensuing discussion, we will only show the construction of the GKS in one dimension. Bear in mind that the GKS is a genuine multidimensional scheme. Since the advection operator in the Boltzmann equation is linear, operator splitting among \( D \) coordinates can be easily implemented. We denote a cell center by \( x, i, j, k \), and its left and right cell boundaries along \( x \) coordinate by \( x_{i-1/2,j,k} \) and \( x_{i+1/2,j,k} \), respectively. For simplicity we set the initial time \( t_0 = 0 \), then the solution (4) at position \( x_{i+1/2,j,k} \) and time \( t \) is,

\[
f(x_{i+1/2,j,k}, t) = e^{-t/\tau} f_0(x_{i+1/2,j,k} - \xi t) + \frac{1}{\tau} \int_0^t f^{(0)}(x', t') e^{-(t-t')/\tau} dt', \quad (6)
\]

where \( x' := x_{i+1/2,j,k} - \xi (t - t') \) is the coordinate of the particle trajectory. In the above equation we omitted the variables in \( f \) which remain unchanged in time. Initially, only the values of the hydrodynamic variables, \( \rho, \mathbf{u} \) and \( \rho E \) are given at the cell center \( x, i, j, k \), but the fluxes are to be evaluated at the cell boundaries \( x_{i \pm 1/2,j,k} = 0 \). Therefore, both \( f_0 \) and \( f^{(0)}(x', t') \) in the above equation are to be constructed from the hydrodynamic variables through the Boltzmann equation and Taylor expansions of \( f \).

We can formally write the BGK equation (2) as

\[
f = f^{(0)} - \tau \partial_t f, \quad \partial_t := \partial_t + \xi \cdot \nabla. \quad (7)
\]

Thus, \( f \) can be solved iteratively, starting with \( f = f^{(0)} \) on the right hand side of the above equation. For the purpose of simulating the Navier-Stokes equation, \( f = f^{(0)} - \tau \partial_t f^{(0)} \) is sufficient. The initial value can
be approximated as
\[ f_0(x, 0) \approx [1 - \tau(\partial_t + \xi \cdot \nabla)]f^{(0)}(x, 0) = [1 - \tau h' \cdot (\partial_t + \xi \cdot \nabla)h] f^{(0)}(x, 0). \] (8)

In addition, the equilibrium can be expanded in a Taylor series about \( x_{i+1/2,j,k} = 0 \),
\[ f^{(0)}(x, 0) \approx [1 + x \cdot \nabla]f^{(0)}(0, 0) = [1 + h' \cdot (x \cdot \nabla)h] f^{(0)}(0, 0). \] (9)

By substituting Eq. (9) into Eq. (8) we have
\[ f_0(x, 0) \approx [1 + h' \cdot (x \cdot \nabla)h] [1 - \tau h' \cdot (\partial_t + \xi \cdot \nabla)h] f^{(0)}(0, 0) = [1 + ax + by + cz - \tau(a\xi_1 + b\xi_2 + c\xi_3 + A)] f^{(0)}(0, 0), \] (10)

where \( a = h' \cdot \partial_x h, b = h' \cdot \partial_y h, c = h' \cdot \partial_z h \) and \( A = h' \cdot \partial_t h \) are functions of \( \xi, \zeta \) and the hydrodynamic variables, \( \rho, u \) and \( T \) and their first order derivatives. They are related by the compatibility condition for \( f \)
\[ \int f^{(n)} \Psi d\Xi = 0, \quad \forall n > 0, \]
where \( f^{(n)} \) is the \( n \)-th order Chapman-Enskog expansion of \( f \), and \( f^{(0)} \) is the Maxwellian of Eq. (9). Therefore, the first-order compatibility condition
\[ \int f^{(1)} d\Xi = -\tau \int dt f^{(0)} d\Xi = -\tau \int (A + a\xi_1 + b\xi_2 + c\xi_3) f^{(0)} d\Xi = 0 \] (11)
leads to the relation between \( A \) and \( a \),
\[ \int A f^{(0)} d\Xi = -\int (a\xi_1 + b\xi_2 + c\xi_3) f^{(0)} d\Xi. \] (12)

In computing the gradients \( \partial_x h, \partial_y h, \partial_z h \) for the coefficient \( a, b, c \) in Eq. (10), we should assume that the hydrodynamic variables can be discontinuous at the cell boundary \( x_{i+1/2,j,k} \) in general.

As for \( f^{(0)}(x, t) \) in the integrand of Eq. (6), it can be evaluated by its Taylor expansion,
\[ f^{(0)}(x, t) \approx (1 + t\partial_t + x \cdot \nabla) f^{(0)}(0, 0) = f^{(0)}(0, 0) [1 + h' \cdot (t\partial_t + x \cdot \nabla)h] \]
\[ = (1 + \bar{a}x + \bar{b}y + \bar{c}z + \bar{A}t) f^{(0)}(0, 0), \] (13)
where \( \bar{a}, \bar{b}, \bar{c} \) and \( \bar{A} \) are similar to \( a, b, c \) and \( A \), respectively. The difference is that in \( \bar{a}, \bar{b}, \bar{c} \) the hydrodynamic variables are assumed to be continuous, but their gradients in \( x \)-direction are not continuous. That means that in \( \bar{a} \) the gradients of hydrodynamic variables are assumed to be discontinuous. The details about how to evaluate \( a, b, c, A, \bar{a}, \bar{b}, \bar{c} \) and \( \bar{A} \) will be discussed next.

Assuming the hydrodynamic variables are discontinuous at the cell boundaries (or interfaces) of \( x_{i+1/2,j,k} = 0 \), then the values of the equilibrium \( f^{(0)} \) on both sides of the cell boundary have to be evaluated differently. For the value \( f^{(0)}_l \) on the left side, the hydrodynamic variables \( h \) are interpolated to the left cell boundary \( x_{i+1/2,j,k}^- \) with two points left and one point right of \( x_{i+1/2,j,k} \), i.e., \( x_{i-1,j,k}, x_{i,j,k} \) and \( x_{i+1,j,k} \). Then the left equilibrium value \( f^{(0)}_l \) is computed from the hydrodynamic variables at \( x_{i+1/2,j,k}^- \). Similarly, the right equilibrium value \( f^{(0)}_r \) is evaluated from the hydrodynamic variables interpolated to \( x_{i+1/2,j,k}^+ \) with two points right and one point left of \( x_{i+1/2,j,k} \), i.e., \( x_{i,j,k}, x_{i+1,j,k} \) and \( x_{i+2,j,k} \). The van Leer limiter is used in the interpolations to suppress the spurious oscillations.\(^6,31\)

Specifically, the gradients of the hydrodynamic variables at the left cell boundary are computed as the following:
\[ \partial_x h_{l}(x_{i+1/2,j,k}) = \frac{h(x_{i+1/2,j,k}) - h(x_{i,j,k})}{x_{i+1/2,j,k} - x_{i,j,k}}, \]
\[ \partial_y h_{l}(x_{i+1/2,j,k}) = \frac{h(x_{i+1/2,j,k}) - h(x_{i,j,k})}{y_{i+1/2,j,k} - y_{i,j,k}}, \]
\[ \partial_z h_{l}(x_{i+1/2,j,k}) = \frac{h(x_{i+1/2,j,k}) - h(x_{i,j,k})}{z_{i+1/2,j,k} - z_{i,j,k}}. \]
Then the coefficient \(a_L, b_L, c_L\) at the left cell boundary \(x_{i+1/2,j,k}^-\) is given by

\[
\begin{align*}
    a_L(x_{i+1/2,j,k}^-) &= h'_L(x_{i+1/2,j,k}^-) \cdot \partial_2 h_L(x_{i+1/2,j,k}^-), \\
    b_L(x_{i+1/2,j,k}^-) &= h'_L(x_{i+1/2,j,k}^-) \cdot \partial_0 h_L(x_{i+1/2,j,k}^-), \\
    c_L(x_{i+1/2,j,k}^-) &= h'_L(x_{i+1/2,j,k}^-) \cdot \partial_2 h_L(x_{i+1/2,j,k}^-).
\end{align*}
\]

Similarly, as for the coefficient \(a_R, b_R, c_R\) at the right cell boundary \(x_{i+1/2,j,k}^+\), the hydrodynamic variables are interpolated from the following three points: \(x_{i,j,k}, x_{i+1,j,k}\), and \(x_{i+2,j,k}\), and we have

\[
\begin{align*}
    \partial_2 h_L(x_{i+1/2,j,k}^+) &= \frac{h(x_{i+1/2,j,k}^+) - h(x_{i+1,j,k})}{x_{i+1/2,j,k} - x_{i+1,j,k}}, \\
    \partial_0 h_L(x_{i+1/2,j,k}^+) &= \frac{h(x_{i+1/2,j,k}^+) - h(x_{i+1/2,j-1,k})}{y_{i+1/2,j+1,k} - y_{i+1/2,j-1,k}}, \\
    \partial_2 h_L(x_{i+1/2,j,k}^+) &= \frac{h(x_{i+1/2,j,k+1}^+) - h(x_{i+1/2,j,k-1})}{z_{i+1/2,j+1,k+1} - z_{i+1/2,j,k-1}}.
\end{align*}
\]

\(a_R, b_R, c_R\) can be calculated in a way similar to \(a_L, b_L, c_L\), except that all the symbols of \(-\) at the superscript of \(x\) in Eq. (15) are replaced by \(+\). With \(a_L, b_L, c_L\) and \(a_R, b_R, c_R\) given, \(A_L\) and \(A_R\) can be obtained immediately by using the compatibility condition (12).

The equilibria at the both sides of the cell boundary \(x_{i+1/2,j,k}\) are \(f(0) := f^{(0)}(\xi, h_L)\) and \(f^{(0)} := f^{(0)}(\xi, h_R)\), which are available now because \(h_L\) and \(h_R\) are given. At equilibrium \(f^{(0)}\), the hydrodynamic variables are assumed to be continuous. Therefore, the conservative variables \(W\) at the cell boundary \(x_{i+1/2,j,k}\) are obtained by integrating the equilibrium at the both sides of the cell boundary:

\[
W(x_{i+1/2,j,k}) = \int_{\xi_s \geq 0} d\Xi \Psi f^{(0)}_L + \int_{\xi_s \leq 0} d\Xi \Psi f^{(0)}_R,
\]

where the hydrodynamic variables \(h := (\rho, u, T)^T\) can be easily obtained from the conservative variables \(W := (\rho, \rho u, \rho E)^T\), then the coefficients \(\tilde{a}_L\) and \(\tilde{a}_R\) are computed as the following:

\[
\begin{align*}
    \tilde{a}_L(x_{i+1/2,j,k}) &= h'(x_{i+1/2,j,k}) \cdot \frac{h(x_{i+1/2,j,k}^+) - h(x_{i,j,k})}{x_{i+1/2,j,k} - x_{i,j,k}}, \\
    \tilde{a}_R(x_{i+1/2,j,k}) &= h'(x_{i+1/2,j,k}) \cdot \frac{h(x_{i+1/2,j,k}^+) - h(x_{i+1,j,k})}{x_{i+1/2,j,k} - x_{i,j,k}}.
\end{align*}
\]

Consequently, we have

\[
\begin{align*}
    f_0(x, t) &= [1 + a_L(x - \tau \xi_1) + b_L(y - \tau \xi_2) + c_L(z - \tau \xi_3) - \tau A_L]H(-x) f^{(0)}(0, 0) + [1 + a_R(x - \tau \xi_1) + b_R(y - \tau \xi_2) + c_R(z - \tau \xi_3) - \tau A_R]H(x) f^{(0)}(0, 0), \\
    f^{(0)}(x, 0) &= [1 + H(-x) \tilde{a}_L x + H(x) \tilde{a}_R x + \tilde{b}_y + \tilde{c}_z + \tilde{A} t] f^{(0)}(0, 0),
\end{align*}
\]

where \(H(x)\) is the Heaviside function. Finally, the value of \(f\) at a cell boundary can be obtained by substituting the above equations of \(f_0(x, t)\) and \(f^{(0)}(x, t)\) into Eq. (6),

\[
\begin{align*}
    f(x_{i+1/2,j,k}, t) &= \left\{\left[1 - \tilde{A} t\right] \left(1 - e^{-t/\tau}\right) + \tilde{A} t \right\} \\
    &\quad + \left\{\left[1 + \tilde{A} t\right] \left(1 - e^{-t/\tau}\right) - \tilde{A} t \right\} \left[\tilde{a}_L H(\xi_1) + \tilde{a}_R H(-\xi_1)\right] \xi_1 + \tilde{b}_x \xi_2 + \tilde{c}_z \xi_3 \right\} f^{(0)}_0, \\
    &\quad + e^{-t/\tau} \left\{\left[1 - (t + \tau) \left(\tilde{a}_L \xi_1 + \tilde{b}_x \xi_2 + \tilde{c}_z \xi_3\right) - \tau A_L\right] H(\xi_1) f^{(0)}_L + \left[1 - (t + \tau) \left(\tilde{a}_R \xi_1 + \tilde{b}_x \xi_2 + \tilde{c}_z \xi_3\right) - \tau A_R\right] H(-\xi_1) f^{(0)}_R\right\},
\end{align*}
\]

where \(f^{(0)}_0, f^{(0)}_L\) and \(f^{(0)}_R\) are initial values of \(f^{(0)}, f^{(0)}_L\) and \(f^{(0)}_R\) evaluated at the cell boundary \(x_{i+1/2,j,k}\). The only unknown in \(f(x_{i+1/2,j,k}, t)\) of Eq. (17) is the coefficient \(\tilde{A}\). By using \(f^{(0)}(x_{i+1/2,j,k}, t)\) of Eq. (16b) and \(f(x_{i+1/2,j,k}, t)\) of Eq. (17), the conservation laws lead to the following equation:

\[
\int_0^\Delta t d\Xi \int f^{(0)}(x_{i+1/2,j,k}, t) = \int_0^\Delta t d\Xi \int f(1+1/2,j,k, t),
\]
which is used to determine $\tilde{A}$ in terms of $a_l$, $b_l$, $c_l$, $a_r$, $b_r$, $c_r$ and $\tilde{a}_l$, $\tilde{b}$, $\tilde{c}$. Therefore, $f^{(0)}(x_{i+1/2,j,k}, t)$ is fully determined from the hydrodynamic variables at the cell centers around the cell boundary $x_{i+1/2,j,k}$.

In Eq. (17), discontinuity has been taken into account. The values of the flow variables and their spatial derivatives on both sides of the cell boundary are evaluated differently due to the assumption of discontinuity. In a smooth flow, however, all the values of the flow variables and their spatial derivatives on both sides of the cell boundary should be approximately equivalent. In such a case, we should have $a_l = a_r = \tilde{a}_l = \tilde{a}_r$, $b_l = b_r$, $c_l = c_r$. As a result, there should be $A_l = A_r = \tilde{A}$ too. Hence, substituting the above relations to Eq. (17) without any further assumption, we can obtain a much simpler gas distribution function at a cell face as follows

$$f(x_{i+1/2,j,k}, t) = f^{(0)}_0 [1 - \tau(a_1 + b_1 + c_1) + t\tilde{A}] + 0.76.$$  

Eq. (18) has been extensively used for the low-Mach-number viscous flow or incompressible flow simulations. In the compressible DHT cases, when the initial turbulent Mach number is not very high (usually less than 0.6), the numerical schemes for smooth flows can generally work well. We find that it is also true for the simplified GKS presented by Eq. (18). In this situation, the macro flow variables and their gradients at the cell boundaries can be computed by using a linear interpolation or other high-order reconstructions depending on the accuracy requirements. When the initial turbulent Mach number is larger than 0.6, the full GKS given by Eq. (17) with the flux limiter has to be used.

The relaxation time $\tau$ in Eq. (17) and (18) needs to be determined in the computation. In the gas-kinetic scheme for compressible flows, the particle collision time is determined by the local macroscopic flow variables through

$$\tau = \mu/p,$$  

where $\mu$ is the dynamic viscosity and $p$ is the pressure. The above relation between $\tau$, $\mu$ and $p$ works well when the flow fields are continuous. When discontinuity is considered as for compressible flows with shocks, one may have to introduce some artificial dissipation to capture shocks. In the GKS method, the artificial dissipation is introduced by modifying the relaxation time $\tau$ as the following:

$$\tau = \frac{\mu(x_{i+1/2})}{p(x_{i+1/2})} + \sigma \Delta t \left(\frac{p_l - p_h}{p_l + p_h}\right) = \tau_0 + \sigma \tau_1,$$  

where $\tau_0$ and $\tau_1$ represent the physical and artificial mean free times, respectively.

In this study, the value of the dynamic viscosity $\mu(x_{i+1/2,j,k})$ in Eq. (19) and (20) is determined by

$$\mu = \mu_0 \left(\frac{T}{T_0}\right)^{0.76} = \mu_0 \left(\frac{\beta_0}{\beta}\right)^{0.76},$$  

where $\mu_0$ and $T_0$ are material-dependent constants, and $\beta := 1/RT$ and $\beta_0 := 1/RT_0$.

In Eq. (20), we use $\tau_0 = \mu/p = \mu/\rho$ to calculate the physical mean free time $\tau_0$, in which the value of $\tau_0(x_{i+1/2,j,k})$ is computed from the values of $T(x_{i+1/2,j,k})$ and $\rho(x_{i+1/2,j,k})$ at the previous time step $t = t_{n-1}$, given by the hydrodynamic variables $h(x_{i+1/2,j,k})$ through $W(x_{i+1/2,j,k})$ of Eq. (15). The term of $\tau_1$, where $\tau_1$ is the artificial mean free time, gives rise to an artificial dissipation, which can be tuned by the parameter $\sigma \in [0, 1]$. The values of pressure evaluated at the left and the right of the cell boundary $x_{i+1/2,j,k}$, $p_l$ and $p_h$, are obtained from $h(x_{i+1/2,j,k}^-)$ and $h(x_{i+1/2,j,k}^+)$, respectively.

With $f$ given at the cell boundaries, the time-dependent fluxes can be evaluated,

$$F_x^{i+1/2,j,k} = \int \xi_x \Psi f(x_{i+1/2,j,k}, t) d\Xi.$$  

So far, we have fully determined the flux $F_x$ through the distribution function $f$ at the cell interface $x_{i+1/2,j,k}$. Following the similar procedure, we can obtain the flux $F_y$ at cell interfaces in other two directions, i.e. $F_y^{i+1/2,k}$ at $x_{i,j+1/2,k}$ and $F_z^{i,j,k+1/2}$ at $x_{i,j,k+1/2}$.

By integrating the above equation over each time step $\Delta t$, we obtain the total fluxes as

$$F_x^{i+1/2,j,k} = \int_0^\Delta F_x^{i+1/2,j,k} dt,$$

$$F_y^{i+1/2,k} = \int_0^\Delta F_y^{i+1/2,k} dt,$$

$$F_z^{i,j,k+1/2} = \int_0^\Delta F_z^{i,j,k+1/2} dt.$$  

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The GKS is an explicit numerical scheme and therefore its time step $\Delta t$ in Eq. (23) is dictated by flow characteristics. For the viscous flows governed by Navier-Stokes equations, the time step can be computed from the following Courant-Friedrichs-Lewy (CFL) conditions:

$$\Delta t \leq \sigma_{\text{CFL}} \frac{\Delta x}{\|u\| + c_s (1 + 2/\text{Re}_\Delta)},$$

where $\sigma_{\text{CFL}}$ is the CFL number, $c_s$ is the speed of sound, $\|u\|$ is the magnitude of the macro flow velocity $u$ and $\text{Re}_\Delta$ is the grid Reynolds number given by $\text{Re}_\Delta = \rho \|u\| \Delta x / \mu$.

Then the flow governing equations in the finite volume formulation can be written as

$$W_{i,j,k}^{n+1} = W_{i,j,k}^n - \frac{1}{\Delta x} (F_{i+1/2,j,k} - F_{i-1/2,j,k}) - \frac{1}{\Delta y} (F_{i,j+1/2,k} - F_{i,j-1/2,k})$$

$$- \frac{1}{\Delta z} (F_{i,j,k+1/2} - F_{i,j,k-1/2}),$$

which are used to update the flow field.

B. Quantities Related with Compressible Decaying Turbulence

In the above numerical strategy, we are actually using the GKS method to simulate the fully compressible Navier-Stokes equations in 3D:

$$\partial_t \rho + \nabla \cdot \rho u = 0$$

$$\partial_t \rho u + \nabla \cdot \rho u u + \frac{1}{\gamma \text{Ma}^2} \nabla p = \frac{1}{\text{Re}} \nabla \cdot \sigma$$

$$\partial_t E + \nabla \cdot E u + \frac{1}{\gamma \text{Ma}^2} \nabla \cdot p u = \frac{1}{\alpha} \nabla \cdot (\kappa \nabla T) + \frac{1}{\text{Re}} \nabla \cdot (\sigma \cdot u)$$

$$\sigma_{ij} := \mu (\partial_i u_j + \partial_j u_i) + \left( \eta - \frac{2}{3} \mu \right) \delta_{ij} \nabla \cdot u, \quad \alpha := (\gamma - 1) \text{Pr \ Re} \text{ Ma}$$

where $\eta = \frac{4}{15} \mu$ is the bulk viscosity coefficient.

The dimensionless parameters for the decaying homogeneous isotropic turbulence (DHIT) are:

$$\text{Re} = \frac{\rho_0 c_{s0} L}{\mu_0}, \quad \text{Ma} = \frac{U}{c_{s0}}, \quad c_{s0} = \sqrt{\gamma RT_0}, \quad \text{Pr} = \frac{\mu_0 c_p}{\kappa_0} = 0.7, \quad c_p = \frac{\gamma R}{(\gamma - 1)}$$

where $\mu_0$ and $T_0$ are determined by initial $\text{Ma}_t$ and $\text{Re}_\lambda$. Note that we do not use any artificial dissipation in the DNS of DHIT, that is, $\sigma = 0$ in Eq. (20).

In this work, we use a domain of size $L^3 = (2\pi)^3$ with periodic boundary conditions in all three directions, and a Cartesian grid of mesh size $N^3$. A divergence-free random initial velocity field $u_0(x)$ is specified with its root-mean-square (rms):

$$u' := \frac{1}{\sqrt{3}} \sqrt{\langle u \cdot u \rangle}.$$  

The initial energy spectrum $E_0(k)$ in the Fourier space $k$ is given by:

$$E_0(k) = A k^4 \exp(-2k^2/k_0^2),$$

where $k = \|k\|$ is the wave number, $A = 1.3 \times 10^{-4}$ and $k_0 = 8$. The initial velocity in $k$-space $\tilde{u}_0(k)$ satisfying the initial energy spectrum $E_0(k)$ is generated according to the procedure due to Rogallo. At $t = 0$,

$$K_0 = \frac{3A}{64} \sqrt{2\pi k_0^5}, \quad \Omega_0 = \frac{15A}{256} \sqrt{2\pi k_0^7}, \quad \varepsilon_0 = 2 \frac{\mu_0}{\rho_0} \Omega_0$$

$$\text{Re}_\lambda := \frac{\langle \rho \rangle \langle u' \lambda \rangle}{\langle \mu \rangle} = \frac{(2\pi)^{1/4}}{4} \frac{\rho_0}{\mu_0} \sqrt{2A k_0^{3/2}}, \quad \text{Ma}_t := \frac{\sqrt{\langle 3u' \rangle}}{\langle \varepsilon_s \rangle} = \frac{\sqrt{3} u'}{\sqrt{\gamma RT_0}}.$$

With $u'$, $\text{Re}_\lambda$ and $\text{Ma}_t$ given at $t = 0$, the initial values of $\rho_0$, $T_0$, and $\mu_0$ can be determined.
The following statistical quantities of turbulence are computed in our simulations:\(^{27,34-37}\)

\[
\begin{align*}
\tilde{E}(k, t) & := \frac{1}{2} \tilde{u}(k, t) \cdot \tilde{u}^\dagger(k, t), \\
K(t) & := \frac{1}{2} \langle \rho u \cdot u \rangle, \\
\varepsilon(t) & := 2 \langle \frac{\mu}{\rho} u \cdot \nabla^2 u \rangle.
\end{align*}
\] (30a)

In addition, we compute the two-point longitudinal velocity difference

\[
\delta u(r|\delta r) := \delta \hat{r} \cdot [u(r) - u(r + \delta r)], \quad \delta \hat{r} := \frac{\delta r}{\|\delta r\|}
\] (31)

and the normal upstream shock Mach number \(Ma_n\):

\[
\frac{\delta u}{c_s} = -\frac{2}{1 + \gamma} \left( Ma_n - \frac{1}{Ma_n} \right).
\] (32)

The shocklet strength \(\chi\) is defined as\(^{24,27,38}\)

\[
\chi := (Ma_n - 1).
\] (33)

We compute the probability distribution functions (PDF’s) of \(\delta u\) and \(\chi\) from the DNS data.

C. Code verification

In the present study, the GKS is going to be applied for the DNS of compressible decaying turbulence. For verification, the GKS has been compared with lattice Boltzmann equation method for the incompressible decaying isotropic turbulence.\(^{22}\) As we know, the LBE has been extensively used for the DNS of incompressible decaying turbulence.\(^{19-21}\) Here we provide one more direct comparison between the current GKS code and the pseudo spectrum method at the near incompressible limit for the decaying isotropic turbulence.

Fig. 1 compares the profiles of the turbulent kinetic energy \(K(t)\) and dissipation rate \(\varepsilon(t)\) obtained from the current compressible code using the GKS and a pseudo spectrum DNS code only for incompressible decaying isotropic turbulence. In order to guarantee the incompressible flow conditions, we set the initial turbulent Mach number \(Ma_t\) very small with the value of 0.1. The Taylor Reynolds number is set to 24 and the computation is performed on the uniform Cartesian grid with the size of \(N^3 = 128^3\). From Fig. 1, the excellent agreement can be found between the GKS and the pseudo spectrum method.

III. Results and Discussions

In this study, we apply the gas-kinetic scheme for direct numerical simulation of compressible decaying homogeneous isotropic turbulence. The grids \(N^3 = 128^3\) and \(256^3\) are used in our simulations. The initial Taylor-microscale Reynolds number is \(Re_\lambda = 72\) so that the flow is well resolved. The initial turbulence Mach number \(Ma_t\) in most cases is between 0.1 and 0.5 and therefore, the GKS presented by Eq. (18) will be used with a linear interpolation at the cell boundaries. We first present the results of the total kinetic energy and the dissipation rate computed with two methods:

\[
\begin{align*}
K_i(t) & := \frac{1}{2} \rho_0 \langle u^2 \rangle, \quad K(t) := \frac{1}{2} \langle \rho u^2 \rangle, \\
\varepsilon_i(t) & := 2 \nu_0 \langle \nabla u \cdot \nabla u \rangle, \quad \varepsilon(t) := 2 \left\langle \frac{\mu}{\rho} u \cdot \nabla^2 u \right\rangle.
\end{align*}
\]

That is, we investigate the effect of density variation on the total kinetic energy and the dissipation rate. As show in Fig. 2 which compares the profiles of the kinetic energy and the dissipation rate obtained by the above two methods for the initial \(Ma_t\) 0.1 and 0.5, the density fluctuation has no visible effect on either the kinetic energy or the dissipation rate. Nevertheless, we consistently use the variable density \(\rho\) in our calculations.
We next investigate the effect of the initial turbulence Mach number $Ma_t$ on the total kinetic energy $K(t)$ and the dissipation rate $\varepsilon(t)$ and the results are shown in Fig. 3. Clearly, the initial turbulence Mach number $Ma_t(0)$ has little effect on the total kinetic energy $K(t)$, however, it has distinct effect on the dissipation rate $\varepsilon(t)$. As the initial turbulence Mach number $Ma_t(0)$ increases, the dissipation rate $\varepsilon(t)$ increases in the initial stage to reach a higher maximum. This effect of $Ma_t(0)$ on $\varepsilon(t)$ is monotonic for $Ma_t(0) \leq 0.5$. This effect will have some significant consequences which shall be discuss later. At the same time, we can see that the change of $Ma_t(0)$ has no visible effect on the asymptotics of $\varepsilon(t)$.

In Fig. 4, we show the initial turbulence Mach number dependence of the dynamics of the Taylor microscale Reynolds number $Re_\lambda(t)$ and the turbulence Mach number $Ma_t(t)$, both normalized by their respective initial values. Clearly, the behavior of $Ma_t(t)$ is similar to that of $K(t)$ with a different decay exponent. However, $Ma_t(0)$ has a strong effect on the dynamics of $Re_\lambda(t)$: the larger $Ma_t(0)$, the faster $Re_\lambda(t)$ decays. This is consistent with the behavior of the dissipation rate $\varepsilon(t)$ shown in Fig. 3, i.e., the larger $Ma_t(0)$, the stronger the dissipation is in the initial stage of the decay process when the decaying cascade is being established.
Figure 3. Effect of the initial turbulence Mach number $Ma_t$ on the total kinetic energy $K(t)$ and the dissipation rate $\varepsilon(t)$. The initial $Re_{\lambda} = 72$ and $N^3 = 256^3$.

Figure 4. Effect of the initial turbulence Mach number $Ma_t(0)$ on the Taylor micro-scale Reynolds number $Re_{\lambda}(t)$ and the dissipation rate $Ma_t(t)$. The initial $Re_{\lambda} = 72$ and $N^3 = 256^3$.

We show next the PDF’s $P(\delta u(\delta r), t)$ of the longitudinal velocity difference $\delta u(\delta r)$, with various values of $\delta r$ and the initial $Ma_t = 0.1$ and $0.5$. For the case of initial $Ma_t = 0.1$, $P(\delta u(\delta r), t)$ for large separation $\delta r$ quickly becomes Gaussian, while the $P(\delta u(\delta r), t)$ with small $\delta r$ remains to non-Gaussian for long time. As for the case of $Ma_t = 0.5$, $P(\delta u(\delta r), t)$ for all values of $\delta r$ becomes Gaussian when $t/\tau > 6.3$, as clearly shown in Fig. 5. These observations demonstrate that at the lower $Ma_t (=0.1)$, intermittency persists; while at higher $Ma_t (=0.5)$, intermittency quickly dies, i.e., $P(\delta u(r), t)$ becomes Gaussian independent of the separation distance $\delta r$.

Finally we investigate the statistics of the shocklet strength. For very large $Re$, the longitudinal velocity difference PDF $P(\delta u(\delta r), t)$ has an exponential tail:

$$ P(\delta u) \sim \frac{1}{\sigma_{\delta u}} \exp \left( -b(r) \left| \frac{\delta u}{\sigma_{\delta u}} \right| \right), \quad \sigma_{\delta u}^2 := \langle (\delta u)^2 \rangle, \quad b(r) = \alpha (r/\eta)^\beta, \quad (34) $$

where $\alpha$ and $\beta$ are constants. With the assumptions that the shock strength $\chi := (Ma_\infty - 1) \ll 1$ and $P(\delta u)$
Figure 5. Effect of the initial turbulence Mach number $Ma_t(0)$ on the PDF of the longitudinal velocity difference $\delta u(\delta r)$, with $\delta r = 1, 2, 4, 8, 16$ and $32$, and in three different times (from left to right). The initial $Ma_t = 0.1$ (top) and $0.5$ (bottom).

of Eq. (34) is uniformly valid for $\delta u < 0$ (weak effect of $Ma_t$),

$$\left| \frac{\delta u}{\sigma_{5u}} \right| = \frac{\sigma^2 \chi^2}{\alpha}, \quad \chi := (Ma_t - 1), \quad \sigma^2 := \frac{4\alpha}{1 + \gamma Ma_t^2},$$

then the PDF of shock strength $\chi$ is given by

$$P_1(\chi) \sim 2\sigma^2 \chi e^{-\sigma^2 \chi^2}.$$ 

(35)

Note that the parameter $\alpha$ determines both the value of $P_1(\chi)$ at $\chi = 0$ and the location of the maximum of $P_1(\chi)$. The most probable shock strength $\chi_{\text{max}}$ given by $P_1(\chi)$ is

$$\chi_{\text{max}} = Ma_t \sqrt{\frac{1 + \gamma}{8\alpha \text{Re}_\lambda}} \iff Ma_{\chi_{\text{max}}} = 1 + Ma_t \sqrt{\frac{1 + \gamma}{8\alpha \text{Re}_\lambda}}.$$ 

(37)

Fig. 6 and 7 present the PDF's for the shocklet strength $\chi$ and the local Mach number $Ma$, respectively, in three times with initial turbulent Mach turbulence Mach number $Ma_t(0) = 0.1, 0.5$ and $2$. Instead of Eq. (18), Eq. (17) with the Van Leer flux limiter is used for the case $Ma_t(0) = 2$ to deal with the discontinuity caused by the strong shocklets. Although $P_t(\chi)$ of Eq. (36) seems to approximately describe the PDF of $\chi$ shown in Fig. 6, it is difficult to find some more from these PDF profiles. Here, we rescale the PDF’s of $\chi$ and $Ma$ such that their maxima are always located at 1 and the corresponding values are also normalized to 1, i.e.,

$$Ma \rightarrow Ma/Ma_0, \quad P_{\text{max}}(Ma_0) = 1,$$

and

$$\chi \rightarrow \chi/\chi_0, \quad P_{\text{max}}(\chi_0) = 1,$$

where $Ma_0$ and $\chi_0$ are the maxima of the PDF profiles of the local Mach number and the shocklet strength, respectively. The rescaled PDF’s of $\chi$ and $Ma$ are shown in Fig. 8.
Figure 6. Effect of the initial turbulence Mach number $M_a(0)$ on PDF’s of the shocklet strength $\chi$. From left to right: The initial $M_a = 0.1$, the PDF of $\chi$ and the PDF of $Ma$ in three times; and the initial $M_a = 0.5$, the PDF of $\chi$ and the PDF of $Ma$ in three times.

Figure 7. Effect of the initial turbulence Mach number $M_a(0)$ on PDF’s of the local Mach number $Ma$. From left to right: The initial $M_a = 0.1$, the PDF of $\chi$ and the PDF of $Ma$ in three times; and the initial $M_a = 0.5$, the PDF of $\chi$ and the PDF of $Ma$ in three times.

Figure 8. Rescaled PDF’s of the shocklet strength $\chi$ (left) and the local Mach number $Ma$ (right).

The rescaled PDF’s of $\chi$ and $Ma$ in Fig. 8 show some interesting features. As for the both cases of $M_a = 0.1$ and $M_a = 0.5$, the PDF’s of the shocklet strength $P(\chi, t)$ in three times all collapse to one single curve, which can be approximately described by $P_1(\chi)$ of Eq. (36). As for the PDF of the local Mach number
Ma, the PDF’s for both Ma = 0.1 and 0.5 and in three times all collapse to the PDF of the initial local Mach number.

IV. Conclusions

In this study, we apply the gas-kinetic scheme for direct numerical simulation of compressible decaying homogeneous isotropic turbulence with different initial turbulent Mach numbers. We present the time evolution of kinetic energy, dissipation rate and the PDF of the two-point longitudinal velocity difference obtained and the PDF of the shocklet strength predicted by the GKS methods. Based on our current DNS results, we make the following observations:

1. With initial Re fixed, increase of initial Ma leads to the increase of ε at the initial stage.
2. Change of Ma has no effect on K(t) and the asymptotics of ε(t).
3. At the lower Ma (=0.1), intermittency persists; while at higher Ma (= 0.5), intermittency quickly dies, i.e., P(δu(r), t) becomes Gaussian independent of the separation distance δr.
4. The PDF’s of both shock strength χ, P(χ, t), and the local Mach number Ma, P(Ma, t) all appear to obey a scaling law.

In our future study, the effect of multi-temperature nonequilibrium on the compressible decaying isotropic turbulence is going to be taken into account and the above observations will be reexamined for the nonequilibrium turbulent gas flows.

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