COMPUTATION OF DECAYING ISOTROPIC COMPRESSIBLE TURBULENCE

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Abstract. The primary aim of this study is to demonstrate the feasibility of the kinetic molecular approach to the problem of turbulence-oriented computation of compressible flow. Particular attention is paid to the feature of decaying isotropic turbulence in 2D and 3D compressible flow cases. The Boltzmann equation in its integral form with the BGK model of the collision term is used. We compare resulting energy spectrum at various time levels with corresponding results of 3D incompressible flow by Yamamoto and Hosokawa (1998) obtained by the Navier-Stokes CFD computation for the Reynolds number $R_e = 200$ and 500 .

Keywords: Turbulence; Molecular kinetic approach; Numerical computation.

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INTRODUCTION

It is increasingly apparent that the molecular kinetic approach is easier to apply than the classical gas dynamics approach for solving some of the problems that are difficult or even impossible to solve by the classic hydrodynamics approach (see e.g.,[1]). Problems with extreme features such as very small structures or very large gradients in the flow field can be considered to be in this category (see e.g., [1], [2] ,[3], [4], [5]).

We consider the problem of computing compressible turbulence. This is known to be not easy to do using the Navier-Stokes code because the ever-finer structure of the flow field causes increasing difficulty by requiring an ever-finer mesh size for larger Reynolds numbers. The feasibility of using molecular kinetic approach to this problem was considered by present authors ([5]), where the Boltzmann equation in its integral form along with the characteristics was used so that one could avoid the finite difference approximation for space derivatives. Note that this integral form is actually, the basis for the Boltzmann equation obtained by making the time interval tend to zero when the conservation law of particle numbers is applied for a short time interval ([6]). Moreover the BGK model was used for the collision term. It is also a very convenient method in computational procedures that involve integration only, thus fewer errors can be expected to accumulate.

As a continuation of the study above we consider here the decaying feature of isotropic compressible turbulence. Many authors have studied this problem in incompressible flows (see e.g., [7]). Following the scheme for these, computations are performed for an initial- value problem of flow with space periodic to a square region for 2D and a cube region for 3D cases to the standard setting as a random initial field with an isotropic energy spectrum. In particular, we set a random initial condition given by a local Maxwellian with a random-phase flow velocity and a magnitude with an isotropic energy spectrum of uniform density and temperature.

BOLTZMANN EQUATION IN INTEGRAL FORM

Consider the Boltzmann equation of two-and three-dimensional molecular gas flows, using a purely two-dimensional model called coplanar flow for 2D cases and a full three-dimensional model for 3D cases. We use coplanar model for 2D for the convenience of comparison of the method with 3D cases, although it would be more realistic to use “Partial moment method” (cf. [8]) for 2D flow to an actual application.

Let the molecular velocity be **c** and the spatial coordinate be **x**. They have two or three components: $\mathbf{c}=(c_x, c_y)$, $\mathbf{x}=(x, y)$ or $\boldsymbol{c}=(c_x, c_y, c_z)$, $\mathbf{x}=(x, y, z)$ respectively, for 2D or 3D cases.

The molecular velocity distribution function f is given as

$$f = f(\mathbf{c}, \mathbf{x}, t). \qquad (1)$$

The function f can be determined from the Bolzmann equation. With use of this, we can avoid the difficulty of finite difference schemes for higher space derivatives such as the one as $\partial^2 u / \partial x^2$ of the Navier-Stokes equation.

Moreover we use its integral form being affected along the characteristic line, or the conservation law on particle numbers for a small time interval Δt expressed without external forces as

$$f(\mathbf{c}, \mathbf{x} + \mathbf{c}\Delta t, t + \Delta t) - f(\mathbf{c}, \mathbf{x}, t) = \Delta t \frac{\delta_e f}{\delta t}, \qquad (2)$$

where $\delta_e f / \delta t$ denotes the rate of change in molecular particle numbers owing to their encounters. As it is mentioned above, Eq.(2) is in fact the basis for the Boltzmann equation, which is indeed obtained by making Δt tend to zero in Eq.(2). The BGK model collision term gives

$$\frac{\delta_e f}{\delta t} = \nu(f_0 - f), \qquad (3)$$

where $\nu = \nu(\mathbf{x}, t)$ is the collision frequency and $f_0 = f_0(\mathbf{c}, \mathbf{x}, t)$ is the local Maxwellian .The equations can be expressed in a dimensionless form based on representative length L, density ρ_0 and temperature T_0. Consequently, we have Eq. (2) and (3) again in the same expression. The macroscopic properties are reduced to

$$f_0 = \frac{\rho}{(\pi T)^{n/2}} e^{-C^2/T}, \quad \mathbf{C} = \mathbf{c} - \mathbf{u}, \quad C = |\mathbf{C}|,$$

$$\rho = \rho(\mathbf{x}, t) = \int f d\mathbf{c}, \quad \mathbf{u} = \mathbf{u}(\mathbf{x}, t) = \frac{1}{\rho}\int f\mathbf{c} d\mathbf{c}, \quad T = T(\mathbf{x}, t) = \frac{1}{\rho}\int \frac{2}{n} C^2 f d\mathbf{c}, \quad p = \rho T,$$

n =2, 3, respectively, for 2D or 3D cases,

where $p, \mathbf{C}, \mathbf{u}, R, c_0$ is pressure, peculiar velocity, mean velocity, gas constant and the most probable molecular thermal speed.

The dimensionless expression of the collision frequency ν depends on molecular model. Here, we use the simplest case of the Maxwellian molecule model (fifth- power law; [6], p.57) to yield

$$\nu = \frac{\rho}{K_n} k_1, \quad k_1 \equiv \frac{8}{5\sqrt{\pi}} = 0.9027, \qquad K_n = \frac{l}{L}, \qquad l = \frac{2k_1\mu_0}{\rho_0 c_0}, \qquad (4)$$

where K_n is the Knudsen number, l the representative mean free path, and μ_0 the representative viscosity coefficient. Let U be the representative velocity and introduce the Mach number *M* and the Reynolds number R_e as

$$M = \frac{U}{c_0}\sqrt{\frac{2}{\gamma}}, \qquad R_e = \frac{\rho_0 UL}{\mu_0},$$

based on ρ_0, L, T_0, μ_0 and γ the ratio of specific heats. We then have the relation

$$K_n R_e = \sqrt{2\gamma} k_1 M. \qquad (5)$$

By introducing the transformation

$$\mathbf{x} + \mathbf{c}\Delta t \to \mathbf{x},$$

in Eq.(2) to give

$$f(\mathbf{c}, \mathbf{x}, t + \Delta t) = f(\mathbf{c}, \mathbf{x} - \mathbf{c}\Delta t, t) + \Delta t \frac{\delta_e f}{\delta t}. \qquad (6)$$

Utilize Eq.(6) to derive the f value at $t + \Delta t$ from data at the time *t*. In practice, we use the approximation in Eq.(6) based on the small time step Δt and the negligibly small f values for large $\mathbf{c}$ values. This results in the following form

$$f(\mathbf{c}, \mathbf{x}, t + \Delta t) = f(\mathbf{c}, \mathbf{x} - \mathbf{c}\Delta t, t) + \Delta t \cdot \nu(\mathbf{x}, t)\{f_0(\mathbf{c}, \mathbf{x}, t) - f(\mathbf{c}, \mathbf{x}, t)\}. \qquad (7)$$

Notice both the similarity and the difference between Eq. (7) and the lattice Boltzmann equation ([7]), which is a discrete model. Notice also its similarity with the formula of the conventional split method for solving kinetic equations (see e.g., [9]) in a sense that the number density change due to the flow and the collision are treated separately. They seem to be almost equivalent in context but are derived from different bases.

For the actual computational work with the values at mesh points, we have to determine the value at $\mathbf{x} - \mathbf{c}\Delta t$ that is not necessarily a mesh point. We, therefore, use a linear interpolation from values at neighboring mesh points consisting of edges of triangle (for 2D) or tetrahedron (for 3D). As usual, computation in $\mathbf{c}$-space is restricted to a finite region $|\mathbf{c}| \le \bar{c}$ with a finite $\bar{c}$ (say) and by assuming $f = 0$ outside. The loss in particle numbers caused by this setting is recovered by the normalization in number density. Integration in $\mathbf{c}$-space is replaced by summations of values at its mesh points in the above finite region.

DECAYING ISOTROPIC TURBULENT FIELD

Now consider the decaying isotropic turbulence, and study an initial value problem for an isotropic turbulent field that is space periodic in a square region for 2D case, and a cubic region for 3D case. A random initial condition is set at time t=0, as is usual practice for this kind of problem. Here a local Maxwellian $f_{00}(\mathbf{x})$ is set with its flow velocity $\mathbf{u}_{00}$, density $\rho_{00} = 1$ and temperature $T_{00} = 1$ for $\mathbf{x} = (x, y, z)$ for 3D or (x, y) for 2D as

$$f_{00} = \frac{\rho_{00}}{(\pi T_{00})^{n/2}} e^{-C^2/T_{00}}, \ \mathbf{C} = \mathbf{c} - \mathbf{u}_{00},$$

where $\mathbf{u}_{00}$ expresses the isotropic fluctuation. For $\mathbf{u}_{00}$, its energy spectrum $E(k)$ is postulated in a same way as that adopted usually for this kind of problem to the incompressible Navier-Stokes equation.

$$E_2(k) = K^2 k^2 \exp\{-(k/k_0)^3\} \quad \text{for 2D}, \qquad E_3(k) = K^2 k^4 \exp\{-2(k/k_0)^2\} \qquad \text{for 3D},$$

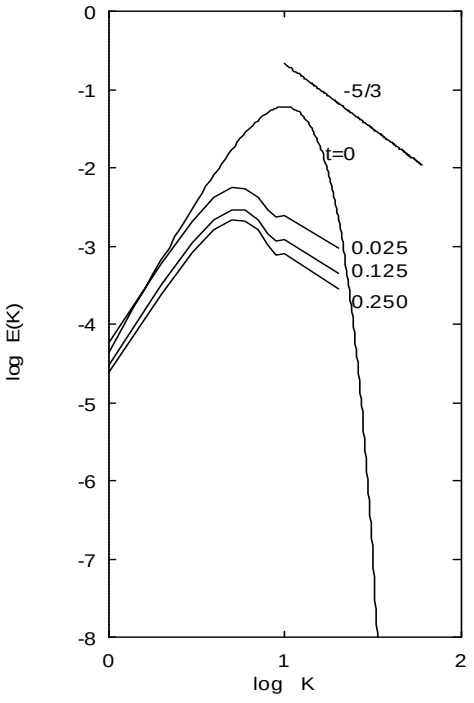
where K is an adjustable constant, and k_0 (the wave number magnitude of energy containing eddies at the initial state) is chosen as $k_0 = 10$. The phase for the individual mode is given randomly for 3D case as follows:

Let $\mathbf{k} = 2\pi\mathbf{n}$, $\mathbf{n} = (n_1, n_2, n_3)$, $n_i = 0, \pm 1, \pm 2, \cdots$ for $i = 1, 2, 3$,

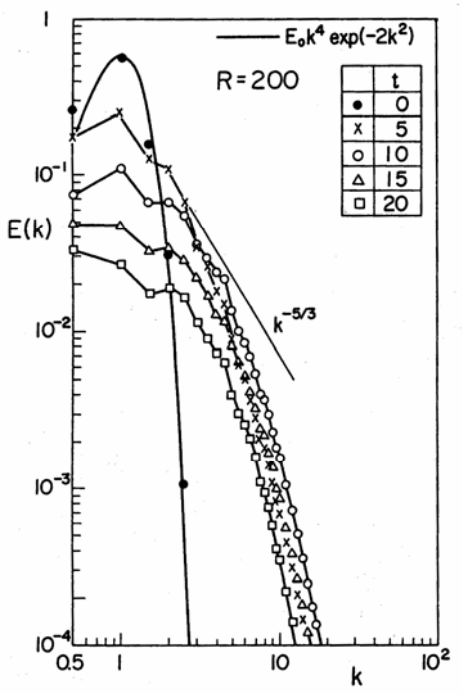
and set

$$\mathbf{u}_{00} = (u_{00}, v_{00}, w_{00}), \ u_{00} = \sum_{\mathbf{n}} a_{\mathbf{n}}(n_1, n_2, n_3) \sin[2\pi\{n_1 x + n_2 y + n_3 z + \varepsilon_{\mathbf{n}}(\mathbf{n})\}], \ a_{\mathbf{n}} = \sqrt{E/k^2},$$

and similar expressions for v_{00} and w_{00}, where $\varepsilon_{\mathbf{n}}(\mathbf{n})$ is random numbers in [0, 1] for each given combination of $\mathbf{n} = (n_1, n_2, n_3)$, $\mathbf{x} = (x, y, z)$ for 3D case, and we have a similar expression for 2D case without w_{00} and n_3. Consider now the present problem of the decaying isotropic turbulent flow, to which K_n value should be less than 0.01 ([10]). Studies on this problem for incompressible flow have been conducted by many authors with use of various DNS schemes for the Navier-Stokes system (see e.g., [7]).



(a)



(b)

FIGURE 1: (a) Energy Spectra at various time levels for $K_n = 0.001, M = 0.12$ $(R_e = 200)$ in 3D computation. (b) Energy spectra at various time levels in a decaying isotropic turbulence in incompressible CFD result for $R_e = 200$ by Yamamoto and Hosokawa (1998).

We consider 3D flows by Yamamoto and Hosokawa (1998,[11]) obtained by spectral method for the initial Reynolds numbers R_e =50～500, and utilize their results to compare the corresponding ones from our kinetic approach to compressible flows. Computations are performed for two 3D cases, K_n = 0.001 and 0.0004 for the scheme above. These K_n values satisfy the criterion of K_n <0.01 for the validity of the solution of the problem, and can be made to correspond respectively to the cases R_e =200 and 500 with a Mach number M of 0.12 by adjusting through the relation of Eq.(5) between R_e , M and K_n with γ =1.4. The representative flow velocity $U = 16Kc_0$ (k_0 =10), accordingly, $M = 19K$ from Eq.(5) for γ =1.4. We have $K = 0.00675$ and computations are performed for time step $\Delta t = 0.125 \times 10^{-3}$, $35 \times 35 \times 35$ divisions for $\mathbf{x}$ and $16 \times 16 \times 16$ for $-1.2 \le c_x, c_y, c_z \le 1.2$ in $\boldsymbol{c}$.

It is noted that the present Boltzmann equation type system is considered to require less divisions in comparison with the one for usual CFD based on the Navier-Stokes equation which is in fact a complex system ([1]), although these data above are not satisfactory enough to provide accurate result. Note also that f -values for molecular velocity beyond 1.2 should be less significant, which is roughly 1.2 times the sonic speed.

The obtained energy spectra at the various time steps are depicted in Fig.1 and Fig.2. Fig.1 (a) depicts for the energy spectra for $K_n = 0.001$ case with $M = 0.12$ ($R_e = 200$) , which is compared with (b) result of CFD computation for the corresponding incompressible flow starting from Reynolds number $R_e = 200$ given in Yamamoto and Hosokawa (1998).

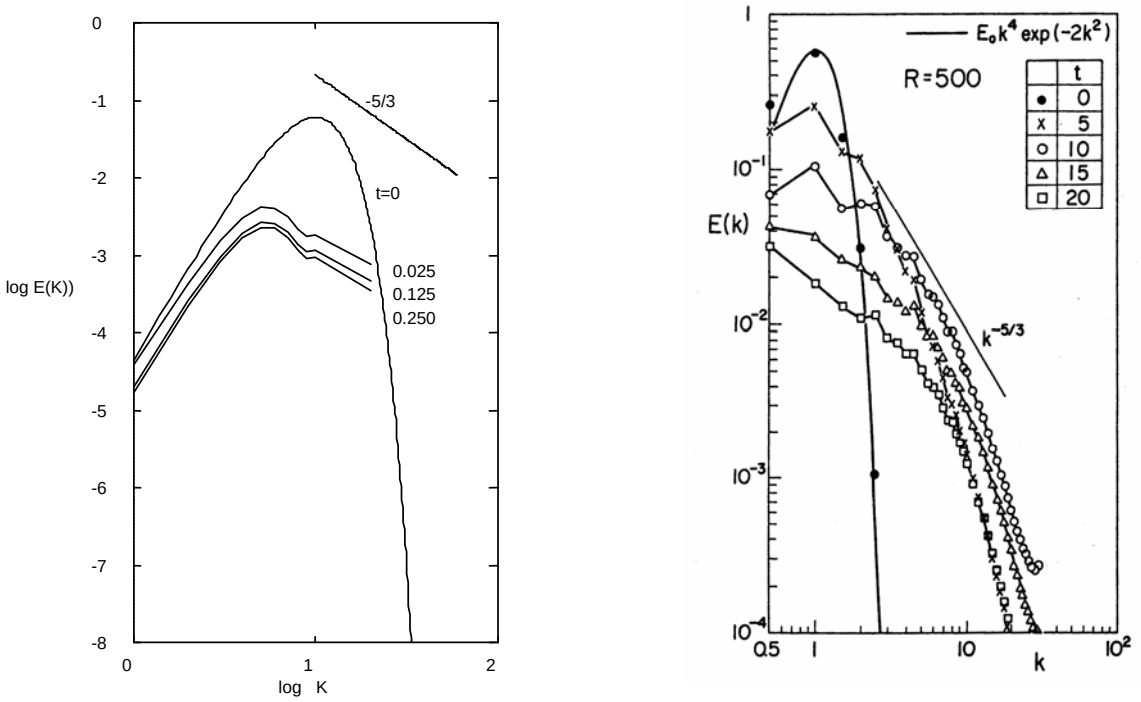
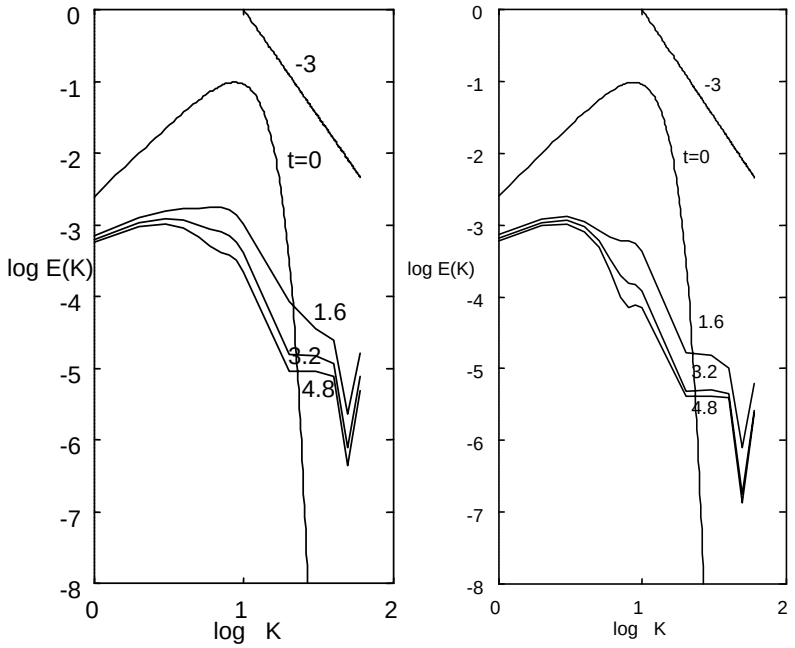


FIGURE 2: (a) Energy Spectra at various time levels for $K_n = 0.0004, M = 0.12$ ($R_e = 500$) in 3D computation. (b) Energy spectra at various time levels in a decaying isotropic turbulence in incompressible CFD result for $R_e = 500$ by Yamamoto and Hosokawa (1998).

Figure 2(a) depicts for the energy spectra for $K_n = 0.0004$ case with $M = 0.12$ and it is compared with (b) for the corresponding incompressible flow starting from Reynolds number R_e =500 given in Yamamoto and Hosokawa (1998). These CFD results as in Fig.1 (b) and Fig.2 (b) for R_e =200,500 are obtained by $128 \times 128 \times 128$ grid points and appear to confirm the characteristics of isotropic turbulence demonstrating the tendency as required for the decaying isotropic turbulence showing a portion in graphs with slope $-5/3$ (cf.

[11]). The above results can also be compared with the more recent results as in Belrtoglio et al (2001, [12]) and Gotoh et al (2002, [13]) for compressible turbulence.

Computation for 2D flow case is performed for K_n=0.001. Time step Δt is 8×10^{-4}. 100×100 divisions for $\mathbf{x}$ and $\Delta c_x = \Delta c_y = 0.5$ for $-5 \le c_x, c_y \le 5$ in $\mathbf{c}$. Computation is started from the Reynolds number R_e=6700 obtained through Eq.(5) with $M = 4.5$ from the maximum value of the initial velocity $U = 62Kc_0$ with $M = 74K$ and the adjusting constant K =0.06. Obtained energy spectra are shown in Fig.3 (a), where energy spectra at various time steps are depicted. They show the tendency as required for the decaying isotropic 2D turbulence having a portion in graphs with the slope of -3. We repeated the 2D computation for the same K_n, R_e values with various combinations of different sizes in $\Delta t, \Delta\mathbf{x}$ and $\Delta\mathbf{c}$ as (1) $\Delta t = 8\times10^{-4}$, 200×200 and $-5 \le c_x, c_y \le 5$ ($\Delta c_x = \Delta c_y = 0.5$) ,(2) $\Delta t = 4\times10^{-4}$, 100×100 and $-5 \le c_x, c_y \le 5$ ($\Delta c_x = \Delta c_y = 0.5$), (3) $\Delta t = 8\times10^{-4}$, 100×100 and $-5 \le c_x, c_y \le 5$ ($\Delta c_x = \Delta c_y = 0.25$). Results of these show some quantitative difference. Result for the case (1) is shown in Fig.3 as Fig.3 (b)



(a) (b)

FIGURE 3: Energy Spectra at various time levels for $K_n = 0.001, M = 4.5$ ($R_e = 6700$) in 2D compu-tation. (a) $\Delta t = 8\times10^{-4}$, 100×100 $-5 \le c_x, c_y \le 5$,($\Delta c_x, \Delta c_y = 0.5$), (b) $\Delta t = 8\times10^{-4}$, 200×200, $-5 \le c_x, c_y \le 5$ （$\Delta c_x, \Delta c_y = 0.5$）.

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