Numerical Simulation of the Eddy System on the Basis of the Boltzmann Equation

V.V.Aristov[a], O.I.Rovenskaya[b]

[a]*Dorodnicyn Computing Centre of Russian Academy of Sciences, Moscow, Russia*
[b]*University of Udine, Udine, Italy*

Abstract. The aim of present work is to investigate the feasibility of applying a kinetic approach to the problem of modeling turbulent or unstable flows. We perform three-dimensional direct numerical simulations of the Taylor Green (TG) type conditions and decay of isotropic turbulence in periodic compressible flow. The simulation is based on the direct numerical solving the Boltzmann kinetic equation. For the regular initial condition the results show the fragmentation of the large initial eddies and subsequently the full damping energy of the system. Dependence of the kinetic energy on the wave number is obtained by means of the Fourier expansion of the velocity components. The decay exponent of the kinetic energy spectrum for both problems close to the value "-5/3".
Keywords: the Boltzmann equation, the Taylor Green condition, isotropic turbulence.

INTRODUCTION

So far turbulence presents different challenges to computational methods, especially for simulation of compressible flows at large Mach numbers. To date, most investigations of instability or turbulence in the literature are based on the continuum Navier-Stokes (NS) equations [1, 2]. In recent times, there has been increasing interest in computing flows with more fundamental kinetic equations for applications involving turbulence and instability which can give another opportunities in comparison with continuum one [3-6]. It was shown that for non equilibrium and unstable processes the utility of the NS equation may be limited due to rarefied gas effects or lack of appropriate constitutive or state relations. These effects can be potentially resolved at the kinetic level of flow description. It is expected that the application of the Boltzmann kinetic equation to the compressible turbulent flows will give more general and correct results. The problem of producing small eddies from large ones in the viscous flow field, which is considered to be one of the basic features of turbulent flows [7]. The kinetic energy exchange appears between eddy structures along with the dissipating energy into a heat. The problem was formulated and examined by Taylor and Green for the incompressible flow using NS equation [8]. In the initial field the series of vortex structures were given and solution was represented in the form of a power series in time. When the flow has a finite Reynolds number, the kinetic energy generated by velocity shear is dissipated by the smallest scales, which provides a simple model for the development of a turbulent flow and the cascade of energy from larger to smaller scales.

STATEMENT OF THE PROBLEM AND NUMERICAL METHOD

We consider 3D gas flow in a periodic domain using the direct numerical solution of the Boltzmann equation:

$$\frac{\partial f}{\partial t} + \xi \frac{\partial f}{\partial \mathbf{x}} = J(f,f) = \int \int_0^{2\pi} \int_0^{b_m} (f'f_*' - ff_*)gbdbd\varepsilon d\xi_* = -v(f)f + N(f,f), \qquad (1)$$

where $f = f(t,\mathbf{x},\xi)$ is the velocity distribution function, $\mathbf{x} = (x, y, z)$ and $\xi = (\xi_x, \xi_y, \xi_z)$, ξ, ξ_*, ξ', ξ_*' are velocities of pair of particles before and after collision, $J(f,f)$ is the collision integral, $\mathbf{g} = \xi_* - \xi$ is the relative velocity, and b, ε are impact parameters, $v(f)f$ is the integral of "direct collisions", $v(f)$ is the frequency of collisions and $N(f,f)$ is the integral of "inverse collisions". In the rest of the paper the non-dimensional formulation of the problem is used and

the scale quantities are the follows: $v_* = \sqrt{RT_*} = v_T / \sqrt{2}$ (v_T is the thermal velocity), the characteristic size of the flow L, effective radius σ_{eff} equals to the radius σ_∞ of hard-sphere particles, characteristic density and temperature n_* and T_* respectively. Thus, non-dimensional variables are $\tilde{\xi} = \xi / v_*$, $\tilde{b} = b / \sigma_{eff}$, $\tilde{\mathbf{x}} = \mathbf{x} / L$, $\tilde{f} = f / (n_* v_*^{-3})$. The initial conditions are given for the non dimensional Maxwell distribution function:

$$f_M(t, \mathbf{x}, \xi) = \rho_0 (2\pi T_0)^{-3/2} \exp\left(-\mathbf{c}^2 / 2T_0\right), \ \mathbf{c} = \xi - \mathbf{V}_0, \ \mathbf{V}_0 = (u_0, v_0, w_0),$$

where ρ_0 is its density, T_0 is its temperature, u_0, v_0, w_0 are its velocities, R is universal gas constant and $\mathbf{x} = (x, y, z)$. TG type initial conditions consist of a first-degree trigonometric polynomial in all directions:

$$u_0(\mathbf{x}) = A\cos(\alpha x)\sin(\alpha y)\sin(\alpha z), v_0(\mathbf{x}) = B\sin(\alpha x)\cos(\alpha y)\sin(\alpha z), w_0(\mathbf{x}) = C\sin(\alpha x)\sin(\alpha y)\cos(\alpha z),$$

$$\rho_0(\mathbf{x}) = 1 + D\sin(\alpha x)\sin(\alpha y)\sin(\alpha z), \ T_0(\mathbf{x}) = 1 + E\cos(\alpha x)\cos(\alpha y)\cos(\alpha z), \tag{2}$$

where $A, B, \dots, E$ are constants, $\alpha = 2\pi$. For a random initial condition density $\rho_0 = 1$, temperature $T_0 = 1$ and magnitudes of velocities u_0, v_0, w_0 obey the isotropic energy spectrum $E(k)$ as [4]

$$u_0(\mathbf{x}) = \sum_n a(n_1, n_2, n_3)\sin 2\pi(n_1 x + n_2 y + n_3 z + \varepsilon), \ a = \sqrt{E / k^2}, \ E = C^2 k^4 \exp^{-2(k/k_0)^2} \tag{3}$$

where $k = 2\pi n$ is wave vector, $k_0 = 10$, $k = |\mathbf{k}|$, $C = \text{const}$ and ε is the random number in [0, 1] for each combination of $n = (n_1, n_2, n_3)$, $n_i = 0, \pm 1, \pm 2, \dots$, $i = 1, 2, 3$. For v_0 and w_0 the expressions are similar to (3). The boundary conditions are $F(\mathbf{x}+1) = F(\mathbf{x})$, for any $F(\mathbf{x})$ of $\mathbf{x}$. The Knudsen Kn, Mach M and Reynolds numbers can be written as

$$Kn = \lambda / L, \ \lambda = 0.5\sqrt{\pi}\mu\sqrt{2RT} / p, \ M = V / a, \ \text{Re} = \rho V L / \mu, \ V = \sqrt{A^2 + B^2 + C^2}, \tag{4}$$

where λ is mean free path, calculated using the expression for the hard – sphere model, μ is dynamic viscosity, p is pressure, R is universal gas constant, $\gamma = 5/3$ is specific heat ratio for monatomic gas, a is the speed of the sound.

To discretize the Boltzmann equation, we introduce a uniform three-dimensional Cartesian grid $\{\xi_\beta\}$ with equidistant nodes in velocity space and a three – dimensional grid $\{\mathbf{x_i}\}$ in physical space. Introducing grid values, the obtained set of equations for $f_\beta(\mathbf{x}, t)$ can be numerically solved using time splitting method, which is obtained considering, in a small time interval $\Delta t = t^{n+1} - t^n$, the numerical solution of the transport step, approximated by a second-order accurate explicit conservative scheme based on the finite volume method (TVD approach):

$$f_{\beta,\mathbf{i}}^{*n+1} = f_{\beta,\mathbf{i}}^{*n} - \Delta t / \Delta\mathbf{x}\left(F_{\beta,\mathbf{i}+1/2}^n - F_{\beta,\mathbf{i}-1/2}^n\right), \ f_{\beta,\mathbf{i}}^{*n} = f_{\beta,\mathbf{i}}^n \tag{5}$$

and the space homogeneous collision step, approximated by an explicit-implicit approach [9, 10]:

$$f_{\beta,\mathbf{i}}^{n+1} - f_{\beta,\mathbf{i}}^n = \Delta t / Kn\sqrt{2}\pi\left(-\nu(f_{\beta,\mathbf{i}}^n)f_{\beta,\mathbf{i}}^{n+1} + N(f_{\beta,\mathbf{i}}^n, f_{\beta,\mathbf{i}}^n)\right), \ f_{\beta,\mathbf{i}}^n = f_{\beta,\mathbf{i}}^{*n+1}. \tag{6}$$

where $\mathbf{i} = (i, j, k)$ and β are indexes in physical and velocity spaces, respectively, $F_{\beta,\mathbf{i}+1/2}^n$ is the numerical flux. For collision integral, written in BGK form, the explicit-implicit scheme approximated the collision step transforms to the implicit scheme since density, velocity and temperature are constant at the uniform relaxation stage

$$(f_{\beta,\mathbf{i}}^{n+1} - f_{\beta,\mathbf{i}}^n) / \Delta t = \tau(\rho_{\mathbf{i}}^{n+1}, \mathbf{V}_{\mathbf{i}}^{n+1}, T_{\mathbf{i}}^{n+1})\left(f_M(\rho_{\mathbf{i}}^{n+1}, \mathbf{V}_{\mathbf{i}}^{n+1}, T_{\mathbf{i}}^{n+1}) - f_{\beta,\mathbf{i}}^{n+1}\right),$$

where τ is the inter collision time. The implicit (or explicit-implicit) scheme is numerically stable, hence allows us to increase Δt and/or evolution time, while introducing the additional approximation error (time derivations of collisions integrals multiplied by $\Delta t / Kn$), thus the accuracy can be increased by decrease in Δt. Generally for the implicit scheme iterations for obtaining the collision integrals at the $(n+1)$-th time level are required, thus the explicit-implicit scheme can be considered as the first iteration of the iterative process. For some situations it is sufficient to use only first iteration, for example, in [5] it has been shown that for the developed turbulent flow (in

the shear layer of the supersonic jet flows) which is low from the kinetic point of view the use of first iteration is sufficient. To understand the character of implicit scheme the series of computation have been carried out using the implicit scheme for the BGK approximation of the collision integral. It was found that results from BGK equation are close to the Boltzmann ones. This gives us an indirect evidence of the adequacy of our approach.

The Godunov method is applied to the linear advection equation for calculation of the numerical flux $F_{\beta,i+1/2}^n$. The second-order accurate scheme (out of extrema and discontinuities) is obtained using the TVD reconstruction procedure with the minmod-type limiter function [11]. The time step is limited by the Courant condition: $\Delta t = CFL \min(\Delta x/ V_{max} + \Delta y/ V_{max} + \Delta z/ V_{max})$, where CFL is the Courant number, V_{max} is a boundary of the velocity space and Δx, Δy and Δz are the mesh sizes in the x, y and z directions, respectively. The quasi - Monte-Carlo method, in which Korobov sequences are used [12], is employed for evaluation of $\nu(f)$ and $N(f,f)$. Generally, the post-collision velocities do not coincide with grid nodes in the velocity space. Therefore, to ensure the execution of conservative laws the procedure of redistribution energy between nearest nodes of the velocity grid (for each collision) is used [13]. This approach provides with microscopic (kinetic) conservation for each collisions. For explicit –implicit scheme the procedure of conservative correction should be applied [9, 10] after collision step. If $g_{\beta,i}^n$ is the solution of (6), then the conservative solution after the relaxation step is defined as:

$$f_{\beta,i}^n = g_{\beta,i}^n(1+P_{\beta,i}^n) = g_{\beta,i}^n(1+a_0 + a_1\xi_x^\beta + a_2\xi_y^\beta + a_3\xi_z^\beta + a_4\xi^{\beta2}), \quad \xi^{\beta2} = \xi_x^{\beta2} + \xi_y^{\beta2} + \xi_z^{\beta2} \; ,$$
$$\sum_\beta \xi_\beta^\alpha f_{\beta,i}^n = \sum_\beta \xi_\beta^\alpha g_{\beta,i}^n, \; \alpha = 0,...,4 \tag{7}$$

where $P_{\beta,i}^n$ is the corrected polynomial, ξ_x^β, ξ_y^β, ξ_z^β are velocity components in the velocity node β. The polynomial coefficients a_0, ..., a_4 are computed from the conservative laws of mass, impulse and energy (7). The correction procedure ensures the positive value of the distribution function after relaxation stage. Therefore, distribution function has acceptable accuracy even if coarse grid is used. Parallelization in physical space is made to improve the efficiency of the algorithm. Each processor is assigned its own set of points in physical space. The relaxation stage is calculated independently on the various processors. Before the stage of the free-molecular transport processors exchange data at neighboring points. The software code was written in C++ with the use of MPI (Message Passing Interface). The calculations have been conducted using multicores system consisted of 2 processes with 4 cores each.

The main indication of the development of vortical cascade is the distribution of kinetic energy $E(q)$ in the wave number space q (q is the wave vector). It is important to determine spectral properties of the flow. To construct the spectrum of the kinetic energy of the flow the following procedure is used [14]. An expansion in Fourier series of the components of velocity vector u_{ijk}, v_{ijk} and w_{ijk}, given on uniform Cartesian mesh, is defined as follows:

$$u_{ijk} = \sum_{l=0}^{N_x-1} \sum_{m=0}^{N_y-1} \sum_{n=0}^{N_z-1} \tilde{u}_{lmn} \cos\frac{\pi l}{L_x} x_{ijk} \cos\frac{\pi m}{L_y} y_{ijk} \cos\frac{\pi n}{L_z} z_{ijk} \; , \tag{8}$$

where $i = 1,…, N_x$, $j = 1,…, N_y$ and $k = 1,…, N_z$ are numbers of the grid, L_x, L_y and L_z are sizes of the computation domain, x_{ijk}, y_{ijk} and z_{ijk} are coordinates in physical space. For v_{ijk} and w_{ijk} the expressions are similar to (8). Each value of the module of the wave vector $q = \sqrt{(l/L_x)^2 + (m/L_y)^2 + (k/L_z)^2}$, $q_{max} = \sqrt{(N_x/L_x)^2 + (N_y/L_y)^2 + (N_z/L_z)^2}$ corresponds to value of kinetic energy $\tilde{E}_{lmn} = (\tilde{u}_{lmn}^2 + \tilde{v}_{lmn}^2 + \tilde{w}_{lmn}^2)/2$ defining by different combinations of $\{l, m, n\}$. The interval $(0, q_{max})$ is divided into p number of the segments each with length $\Delta q = q_{max}/p$. Corresponding values of E_{lmn} are summarized in each segment. The constructed in this way function is considered as a spectral characteristic of the flow field obtained by numerical modeling. The spectral function well describes all scales for $p = 36$, for larger p in the area of moderate and small scales the oscillations appear, possibly due to trigonometric factor.

3D TAYLOR –GREEN PROBLEM

Here we consider the 3D case represented by initial condition (2) and boundary conditions (4). We investigate several cases with the following initial amplitudes and different rarefaction: $A = 0.5$, $B = C = -0.2$, $D = E = 0.01$ for $Kn = 0.01$, $Kn = 0.005$ and $Kn = 0.0025$. Reynolds numbers varies from 63.8 to 255.3 respectively. For all cases the grid in the unit cube is $40 \times 40 \times 40$, velocity space is limited by $V_{max} = 5$ and the step in velocity space is $\Delta\xi = 0.55$.

The time step is chosen in such way that the particle does not pass the distance more than mean free paths and to avoid time step effect: $\Delta t = 2 \times 10^{-3}$ for $Kn = 0.01$, $\Delta t = 10^{-3}$ for $Kn = 0.005$ and $\Delta t = 5 \times 10^{-4}$ for $Kn = 0.0025$. The CPU time was about 128 h (for $Kn = 0.01$) for fully damp flow until $t = 1$. In the Fig. 1 (*a, b*) the iso-surface and contours on the plane $z = 0.5$ of density and module of vorticity vector $\boldsymbol{\omega} = \nabla \times \mathbf{v}$ at the several time moments are shown. At the initial time moment macroparameters demonstrates the constant number of iso-surfaces.
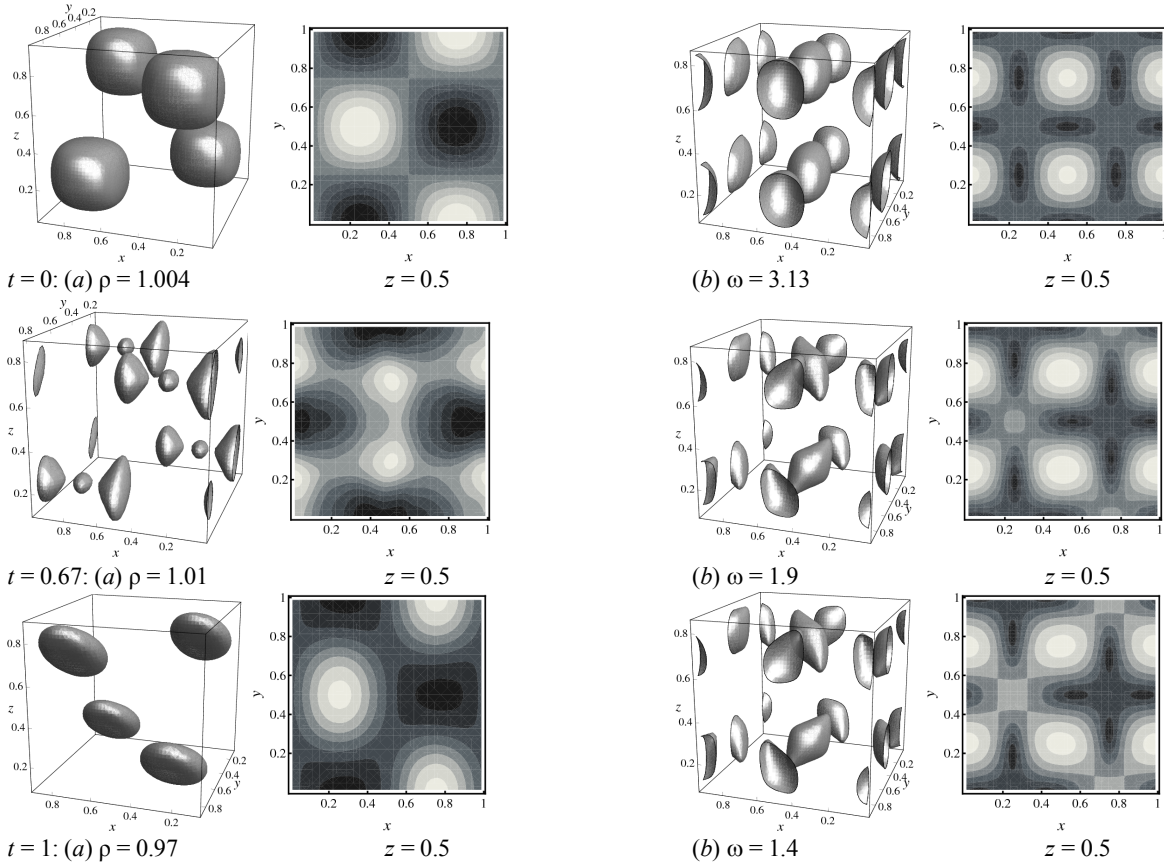

FIGURE 1. Iso-surfaces and contours on the plane $z = 0.5$ of density (*a*) and vorticity (*b*) at $t = 0, 0.67$ and 1 for 3D TG flow with $A = 0.5$, $B = C = -0.2$, $D = E = 0.01$ and $Kn = 0.01$.
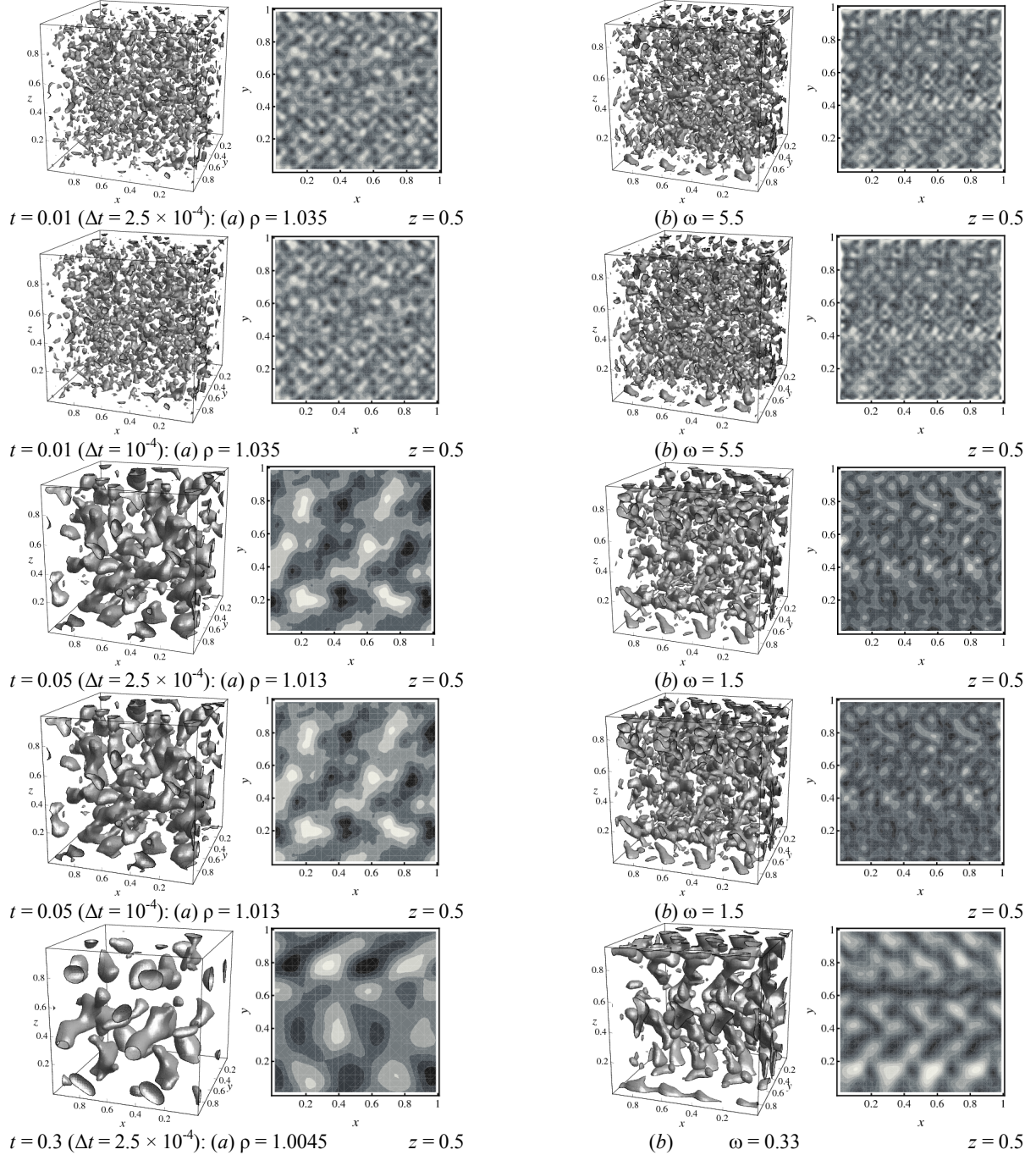
With time growth small scales appears, nevertheless from some time moment ($t > 0.67$) iso-surfaces of the flow parameters remain quasi constant (Fig. 1). In Fig. 3 *a* changing of energy spectra is shown at several time moments $t = 0.25, 0.67$ and 1. The initial kinetic energy monotonous decays with time due to the absence of external sources and energy transfer from kinetic to internal modes due to viscous action. Nevertheless, at all time level spectrum demonstrates the slope "-5/3" for the inertial interval, corresponding the isotropic turbulence power law characteristic [15]. Spectrum of the kinetic energy for smaller Knudsen number is larger. Of course this case is far from isotropic turbulent state, but demonstrates a main feature of turbulence the forward cascade.
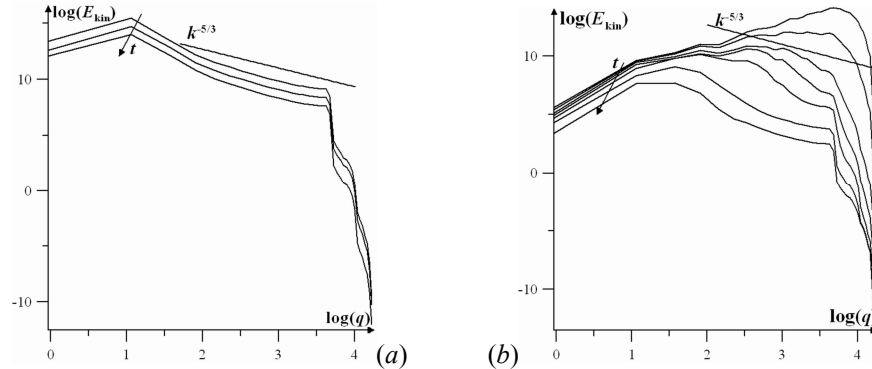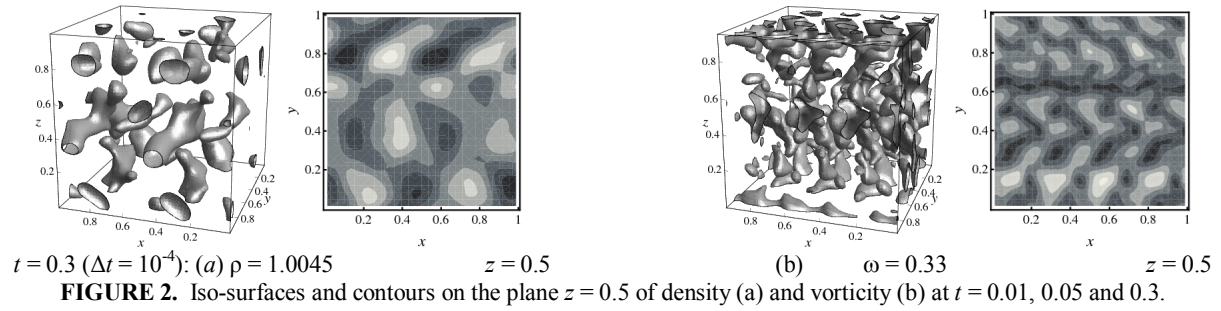
ISOTROPIC TURBULENT FIELD

3D decaying turbulence in the space periodic cube with the initial condition given by a local Maxwellian with a random – phase flow velocity (3) and a magnitude having an isotropic energy spectrum with $C = 0.05$, and a uniform density and temperature are considered. Knudsen, Mach and Reynolds numbers are $Kn = 0.001$, $M = 0.584$ and $Re = 963$ respectively. $40 \times 40 \times 40$ division in the unit cube is set and velocity space is restricted to $V_{max} = 5$, a velocity step size is $\Delta \xi = 0.55$. Computations have been carried out with $\Delta t = 10^{-3}$, 2.5×10^{-4} and 10^{-4} to assess time step effect. Comparison of iso-surfaces of the density ρ and modules of vorticity ω and their contours on the plane $z = 0.5$ (see Fig. 2) computed with last two time steps at various time levels shows that the difference between results is negligible. Fig. 2 demonstrates that the density distribution changes quickly to a turbulent state from the initial uniform state. At a relative small time the both figures of the density and vorticity distributions show patterns close

to the turbulent state. With time growth small scales join to each other and vortices become fewer. They are larger and sparser in space, and they undergo less frequent close encounters. Since those close encounters are the occasions when the vortices change through deformation in ways other than simple movement, the overall evolutionary rates for the spectrum shape and vortex population become ever slower, even though the kinetic energy does not diminish.

An analysis of spectra, presented in Fig. 3 *b*, shows there are number of points lay on the lane with inclination "-5/3", as expected for the inertial interval of 3D isotropic turbulence [15]. After this interval graph of kinetic energy drops sharply. With time growth the inertial interval of wave numbers increases.

$t = 0.01$ ($\Delta t = 2.5 \times 10^{-4}$): (*a*) $\rho = 1.035$ $z = 0.5$ (*b*) $\omega = 5.5$ $z = 0.5$

$t = 0.01$ ($\Delta t = 10^{-4}$): (*a*) $\rho = 1.035$ $z = 0.5$ (*b*) $\omega = 5.5$ $z = 0.5$

$t = 0.05$ ($\Delta t = 2.5 \times 10^{-4}$): (*a*) $\rho = 1.013$ $z = 0.5$ (*b*) $\omega = 1.5$ $z = 0.5$

$t = 0.05$ ($\Delta t = 10^{-4}$): (*a*) $\rho = 1.013$ $z = 0.5$ (*b*) $\omega = 1.5$ $z = 0.5$

$t = 0.3$ ($\Delta t = 2.5 \times 10^{-4}$): (*a*) $\rho = 1.0045$ $z = 0.5$ (*b*) $\omega = 0.33$ $z = 0.5$

$t = 0.3$ ($\Delta t = 10^{-4}$): (*a*) $\rho = 1.0045$ $z = 0.5$ (b) $\omega = 0.33$ $z = 0.5$

FIGURE 2. Iso-surfaces and contours on the plane $z = 0.5$ of density (a) and vorticity (b) at $t = 0.01$, 0.05 and 0.3.

FIGURE 3. Energy spectra $E_{kin}(q)$ (*a*) for 3D TG flow with $A = 0.5$, $B = C = -0.2$, $D = E = 0.01$ at $t = 0.25$, 0.67 and 1 and $Kn = 0.01$, (*b*) for decaying isotropic turbulence at $t = 0$, 0.01, 0.03, 0.05, 0.1, 0.5 and 1.

CONCLUSIONS

The direct numerical solution of the Boltzmann equation based on an explicit-implicit approach was used to analyze the long time evolution of the viscous compressible weakly rarefied gas. Two kind of the initial conditions (TG and random velocity types) were considered. The development of initial state was demonstrated through the kinetic energy distribution. On the kinetic level considered process of energy transfer from large scales to small ones and sequential energy dissipation to heat. Moreover, computation for the space periodic flow started from a random velocity and uniform density and temperature exhibited a flow field pattern close to isotropic turbulence at the initial time moment. Discovered an inertial interval with the exponent "-5/3", predicted for 3D isotropic turbulence, which growths with time.

REFERENCES

1. D. Drikakis, C. Fureby, F.F. Grinstein and D. Youngs, *Journal of Turbulence*, **8**, 1-12, (2007).
2. R. Samtaney, D.I. Pullin and B. Kosovic, *Physics of Fluids*, **13**, 1415–1430 (2001).
3. G.A. Bird, "The Initiation of Centrifugal Instabilities in an Axially Symmetric Flow in *20th Symposium on Rarefied Gas Dynamics*, edited by C. Shen, Peking University Press, Beijing, China, 1997, pp. 149-154.
4. A. Sakurai, and F. Takayama, *Physics of Fluids*, **15**, 1282–1293 (2003).
5. V.V. Aristov, *Comput. Math. Math. Phys.*, **44**, 1069-1081 (2004).
6. O.I. Rovenskaya. *Comput. Math. and Math. Phys.*, **47**, 1544 – 1550 (2007).
7. G.K. Batchelor, *The Theory of Homogeneous Turbulence*, Cambridge: Cambridge Univ. Press, 1971.
8. G.I. Taylor and A.E. Green, *Proc. R. Soc. London Ser. A*, **158**, 495-498 (1937).
9. V.V. Aristov, *Methods of Direct Solving the Boltzmann Equation and Study of Nonequilibrium Flows*, NY: Springer, 2001.
10. V.V. Aristov, F.G. Tcheremissine, *USSR Comp. Math. Math. Phys.*, **20**, 190-225 (1980).
11. A.G. Kulikovskii, N.V. Pogorelov, and A.Yu. Semenov, *Mathematical Aspects of Numerical Solution of Hyperbolic Systems*, Moscow: Fizmatlit, 2001.
12. N.M. Korobov, Exponential Sums and Their Applications, New York: Springer-Verlag, 1992.
13. F. Tcheremissine, "Direct Numerical Solution Of The Boltzmann Equation " in *24th Symposium on Rarefied Gas Dynamics*, edited by M. Capitelli, AIP Conference Proceedings 762, American Institute of Physics, Melville, NY, 2005, pp. 677-685.
14. S.M. Garina, N.V. Zmitrenko, M.Ye. Ladonkina, I.G. Lebo1, V.V. Nikishin, N.G. Proncheva, V.B. Rozanov', V.F. Tishkin, *Mathematical modeling*, **15**, 3-11, (2003)
15. A.N. Kolmogorov, *J. Fluid Mech.*, **13**, 82-85, (1962).