# On Evolution of Vortical System in Rarefied Gas Flow

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**Abstract.** The problem on vortical rarefied gas flow evolution with the Taylor-Green initial conditions and the periodic boundary conditions in two-dimensional case is considered. To solve this problem the direct simulation Monte-Carlo method is used. Results of numerical simulation allow to trace the initial stage of vortical flow development and to define spectral properties of the flow.

## INTRODUCTION

The main task of the turbulence theory is to study general dynamics and the nature of fluid turbulent motion, i.e., investigate dynamics of flow structures and statistically represent the turbulent motion [1]. Vortex dynamics is a natural paradigm for study of chaotic fluid fields and dynamical systems. In this connection, the problem of energy spectrum formation in turbulent flows is of great interest [1, 2]. It is well known that sizes of small eddies in turbulent flows exceed the mean free path in a gas by 2-3 orders of magnitude [3]. This means that study of cascade vortical phenomena in rarefied gas flows is an important problem.

Numerous theoretical and experimental studies of turbulent flows have been made up to the date; the major part of them is devoted to definition of spectral laws for turbulent flows [1, 4, 5]. From the theoretical viewpoint the distribution of turbulent kinetic energy spectral density in the wave-number space is a primary characteristic of developing turbulence. Detailed properties of flows can be obtained by the means of numerical simulation [2, 3, 6, 7]. Despite the fact that the direct numerical simulation (DNS) is limited by computational resources, it allows considering homogeneous as well as non-homogeneous turbulent flows of different nature [3, 6, 7]. In the first case, the choice of initial conditions plays an important role [6]. An interesting class of turbulent flows is two-dimensional flows. Such flows can be observed in the nature [5], their analysis can give a better understanding of turbulent motion. In the present work the problem on the energy cascade formation for specific two-dimensional flow is considered. The Taylor-Green initial conditions [8] and the periodic boundary conditions are used. The problem solution is obtained with the direct simulation Monte-Carlo (DSMC) method [9]. The data obtained are compared qualitatively with those from Ref. [6].

## PROBLEM STATEMENT

Consider the problem on the vortical rarefied gas flow evolution with the Taylor-Green initial conditions and the periodic boundary conditions. Remark that this problem can be viewed as a model for the homogeneous decaying turbulence [8]. The same problem was investigated in [6] using other kinetic models.

At the time instant $t = 0$ the initial conditions in the form of distributions of dimensionless velocity components, density and temperature specified as

$$\begin{aligned} u_{t=0}(x,y) &= A\sin(2\pi x)\cos(2\pi y)\,, \\ v_{t=0}(x,y) &= B\cos(2\pi x)\sin(2\pi y)\,, \\ n_{t=0}(x,y) &= 1 + C\sin(2\pi x)\sin(2\pi y)\,, \\ T_{t=0}(x,y) &= 1 + D\cos(2\pi x)\cos(2\pi y)\,, \end{aligned} \qquad (1)$$

where $A = 0.5$, $B = -0.4$, $C = D = 0.1$. The computational domain is the unit cube: $0 \le x \le 1$, $0 \le y \le 1$, $0 \le z \le 1$. The periodic boundary conditions are imposed on all sides of the computational domain: $F(x + 1, y+ 1, z+ 1) = F(x, y, z)$. The initial conditions correspond to the compressible subsonic flow case, $M_{max} = 0.39$ is the maximal Mach number in the initial field, $Kn_0 = 0.007$ is the Knudsen number for the undisturbed gas state, $Re = \sqrt{\gamma\pi/2}\, M/Kn$ is the Reynolds number, $Re_{max} \cong 90$. We consider a monatomic gas and the hard spheres collisional model is used.

During the development of the initial flow field, formation of smaller structures from larger ones occurs with the kinetic energy transfer to smaller scales and subsequent energy dissipation to the heat. These are essential features of the turbulent flow. Distributions of flow parameters at sequential time instants and the dependence of the kinetic energy spectral density from the wave number are discussed in the context of vortical dynamics characteristics.

## NUMERICAL METHOD PECULIARITIES

Herein we describe main features of the DSMC method for the purpose of clarification of methodical aspects affecting the problem solution. The DSMC method splits the evolution of a gas, described by the Boltzmann equation, into spatially uniform relaxation and collisionless transition using a sequence of small time intervals $\Delta t$. It is assumed that the physical space is discretized with a computational grid sufficient for resolution of the kinetic scales. The boundary conditions are taken into account at the transition stage. In this problem they are realized by the periodic transformation of coordinates of a particle intersecting a boundary.

Numerical realization of the collisional relaxation in the $N$-particle system in a cell is usually based on the majorant frequency scheme. This scheme uses the majorant $\nu_m$ of the collision frequency $\nu(\mathbf{C})$, where $\mathbf{C} = \{\boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_N\}$ is the $3N$-dimensional velocity vector [9, 10]. The initial estimate of the majorant $\nu_m$ for the hard spheres collisional model is

$$\nu_m = N g_{\max} / (2^{3/2} \lambda) = N g_{\max} / (2^{3/2} \mathrm{Kn}\, L),$$

where $\lambda = 1/(\sqrt{2} n \sigma)$ is the local mean free path, and $g_{\max} \sim \sqrt{RT}$ is the maximal relative velocity. The time $\tau$ that separates collisions within the time interval $\Delta t$, is calculated in accordance with the Poisson distribution:

$$\tau = -\nu_m^{-1} \ln \alpha .$$

The value of $\tau$ is added to a counter, and under the condition $\Sigma\tau \le \Delta t$ the collision is calculated as follows. First, a pair of particles with velocities $(\boldsymbol{\xi}_i, \boldsymbol{\xi}_j)$ is equiprobably selected from $N(N–1)/2$ pairs. Second, if $\beta \le g_{ij}/g_{\max}$, their velocities are changed in accordance with the conservation laws. Otherwise, if $\beta > g_{ij}/g_{\max}$, the collision is viewed as fictitious and their velocities remain unchanged. Here $\alpha$ and $\beta$ are independent random numbers uniformly distributed on the interval (0, 1). If $g_{ij} > g_{\max}$, it is necessary to set $g_{\max} = g_{ij}$ and to recalculate the collision. The majorant frequency scheme is computationally effective and accurate for the master kinetic equation describing the spatially uniform relaxation in the $N$-particle system [10].

The time step $\Delta t$ should be chosen from the Courant-like condition, according to which the major part of particles should be transferred in space during $\Delta t$ at a distance not exceeding the local cell size. The Courant condition and the spatial kinetic scales resolution condition guarantee resolution of flow time scales, this also means that repeated collisions do not affect the numerical solution [11]. The necessary number of modeling particles in a cell and consequently the number of independent statistical realizations can be estimated from the condition of equality between the statistical error $\delta_s \sim \sqrt{T}/\sqrt{N}$ and the discretization error $\delta_d \sim O(\Delta t, \Delta x)$, where $T$ is the temperature, $N$ is the total number of particles in a cell.

Calculations were conducted using the dimensionless variables that are obtained with the following scales: the velocity scale $c = \sqrt{RT_{ref}}$, the length scale $L$ and the time scale $\tau = L/c$, where $T_{ref}$ is the reference temperature of undisturbed gas, $L$ is the domain size. A uniform spatial grid with dimensions 110×110×1 is used. The time step $\Delta t$ corresponds to the condition $CFL = 0.5$. In every statistical realization, $N = 75$ particles represent the unit dimensionless density in a cell. After 416 independent statistical realizations, the total number of particles per cell was driven up to 31 200. The algorithm is implemented in the C++ language and uses the MPI parallel library. Calculations were conducted using the MVS-1000/16 system; the total CPU time equals approximately 5700 hours.

## MODELING RESULTS

Characteristics of the developing vortical flow with the initial conditions (1) are considered at sequential time instants $t = 0$, $t = 0.1$ and $t = 0.2$. The initial density field at $t = 0.1$ is shown in Fig. 1. The density fields obtained using the DSMC method are shown in Fig. 2 for $t = 0.1$ and $t = 0.2$. In order to compare the DSMC results with the continuum solution, we use the Euler equations numerical solutions. These are obtained using the second-order accurate finite-difference method [12]. In this case, spatial grids with dimensions 100×100, 200×200, 400×400 are used. The density fields at $t = 0.1$ and $t = 0.2$ obtained with 200×200 grid are shown in Fig. 3.

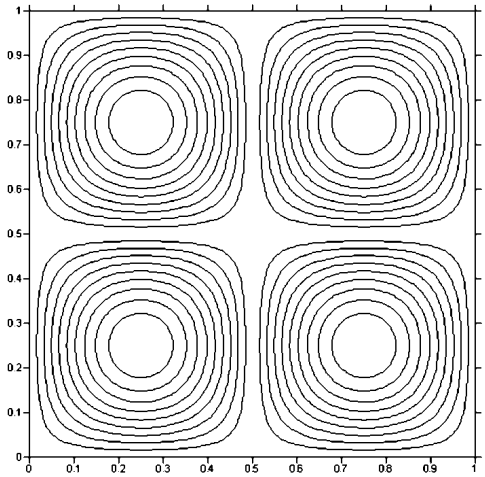


**FIGURE 1.** Isolines of the density field at $t = 0$.

Sequential density distributions show the system of eddies development with the production of smaller structures. In the process of evolution, the energy exchange between eddies occurs along with the loss of energy by eddies and their gradual destruction. In both rarefied gas and continuum cases, the density distributions turned out to be similar in general. This means that large eddies dynamics can be described by the Euler equations within time interval of the order of characteristic vortex time. This statement is not correct applied to small eddies, which are more subjected to the dissipation. A methodical sense of such comparison is to show that the vortical pattern in a compressible gas is defined mainly by the non-barotropy mechanism captured by the Euler equations.

Under the assumption of homogeneous isotropic turbulence, characteristics of Fourier spectra of random fields do not depend on the wave vector direction; therefore the spectrum can be found using one direction. The spectral density of kinetic energy for the isotropic turbulent flow can be defined as $E_k = E(\mathbf{k})/2\pi k$, where $E(\mathbf{k})$ is the two-dimensional spectral density. If the Reynolds number is not large, and the initial conditions are not scale-representative, the assumption of isotropic turbulence is not fully correct. For this reason some representative directions are chosen and the averaging of data is performed [6]. Note that the numerical data obtained with the DSMC method are «noisy» due to fluctuations; therefore the use of discrete Fourier transformation can give incorrect values of short waves spectral amplitudes. The way to resolve this problem is to find the Fourier amplitudes $E_k$ as coefficients obtained with the least-squares method using predefined set of trigonometric functions.

Distributions of the kinetic energy spectral density at $t = 0.2$ obtained with the DSMC method and with the finite-difference method are presented in Fig. 4. The distributions at $t = 0.1$ are found to be similar to those at $t = 0.2$; this indicates that the spectrum is formed up to this stage. As it was already stated, the flow cannot be considered as the developed turbulent flow: the inertial range is rather narrow and the result is mainly qualitative. Figure 4 shows that the main part of the kinetic energy is contained in large eddies. The spectral curve constructed in logarithmic coordinates has a slope close to «–3» in the range of wave numbers $1.7 < \log(k) < 2.2$. This range can be identified as the inertial interval of the energy transfer from small wave numbers to large ones under the assumptions of qualitative theory of the isotropic turbulence [4]. The Euler spectral curve agrees well with the DSMC spectral curve up to $\log(k) = 1.7$; it is fast damping at $\log(k) > 2$ due to the short-wave disturbances suppression by the TVD schemes. The DSMC spectral curve has a slope close to «-1» for larger wave numbers ($\log(k) > 2.25$); this phenomenon is related to statistical fluctuations.

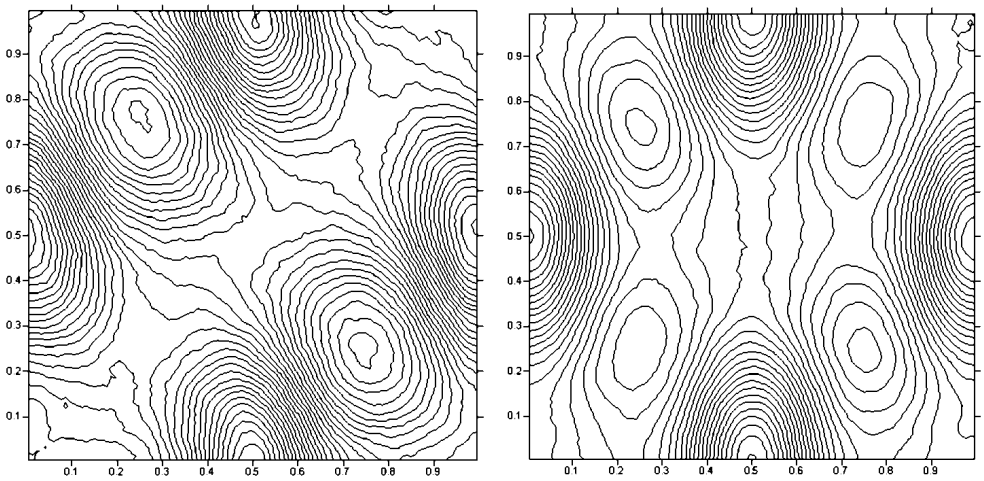


**FIGURE 2.** Isolines of the density fields at $t = 0.1$ и $t = 0.2$, obtained with the DSMC method.

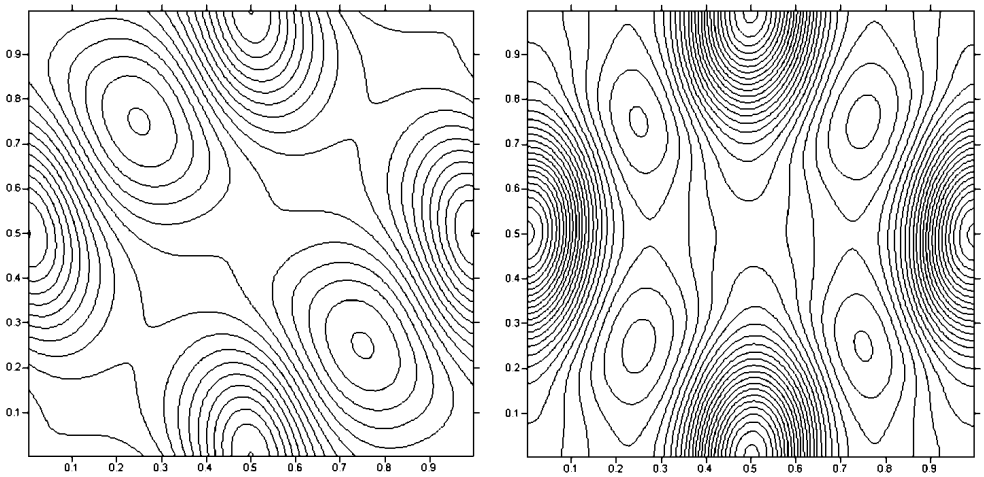


**FIGURE 3.** Isolines of the density fields at $t = 0.1$ и $t = 0.2$, obtained with the finite-difference method.

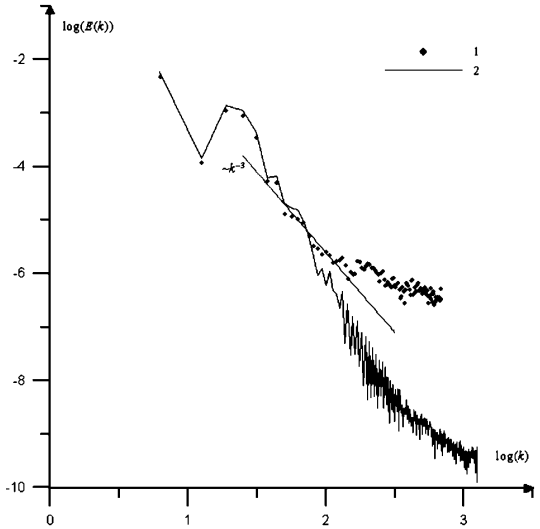


**FIGURE 4.** The spectral density of the kinetic energy at $t = 0.2$: 1 – solution, obtained with the DSMC method, 2 – solution, obtained with the finite-difference method.

## CONCLUSIONS

In the present work the spectral characteristics of the evolving vortical rarefied gas flow are examined using the DSMC method. The inertial range, characterized by the $E(k) \sim k^{-3}$ law for the kinetic energy spectral density is confirmed. This result agrees with theoretical ideas and other numerical results [1, 4, 6]. Although we have not the developed turbulence with wide range of scales, the compressible turbulent flow features, such as the formation of new scales and the energy cascade, are observed. Note that there are experimental confirmations of the $E(k) \sim k^{-3}$ spectral law for nearly two-dimensional flows, i.e., spectra obtained from measurements in thin soap films have the inertial range characterized by this law [5].

The method of parallelization based on independent statistical realizations is suitable for the problem considered. Its using for the simulation of bifurcation phenomena (for example, vortex structures creation as a result of flow instability [3]) requires careful examination of the statistical error influence on the flow pattern.

Our work serves a purpose of better understanding of the turbulent motion nature using the direct numerical simulation.

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