3D numerical simulation of molecular clouds collision process

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Abstract.
We represent results of numerical simulation of molecular clouds dynamical collision. The problem was considered in 3D on extremely high resolution computational grids. The choice of so highly detailed grids is necessary due to fulfillment of numerical Jeans instability. The numerical code was parallelized using OpenMP and CUDA. The code uses Automatic Mesh Refinement (AMR) procedure. We discuss the application of the used numerical method for the simulation of molecular clouds fragmentation, formation of proto-cores and filaments formation what is important for the star formation processes.

1. Introduction

The Interstellar matter (ISM) which consists of the gas and dust contains about 10 − 15% of galactic disc total mass [1]. ISM is significantly non-homogeneous. The density in some ISM regions can have rather large density. The reasons of formation of such non-homogeneities are different, but such clumps are qualitatively differ from other ISM. When molecular clouds(MC) merge or when shock waves pass through the MC the gas in MC could be contracted by many orders. It can lead to the fragmentation and restructuring of the clouds. As the result of such processes a system of dense filaments is formed. At relatively small scales (about 1 parsec) in numerous dense cores in the filaments star formation processes take place.

The resulting turbulent movements become the dominant factor in the formation of regions of gas with increased density, some of which could become protostars. This leads to gravitationally bound systems, which eventually collapse into new stars. The bulk of the clouds are scattered as a result of the transfer of some of the kinetic energy of the incident shock wave. The Fig. 1 is an example of a collision of two molecular clouds, which is the triggering mechanism for the formation of new stars [2].

In the paper we represent the results of the numerical simulation of MC collision processes. Turbulent motions which appear during the collision is a dominating reason for the formation of regions with increased density part of which could became protostars. Some parts of the clouds are scattered as a result of the transfer of some of the kinetic energy of the incident shock wave.

A number of researches have been devoted to the study of the behavior of molecular dust clouds and the study of their role in the formation of stars. In pioneering works [3, 4], the
processes of interaction of flows with various inhomogeneities were studied analytically. Problems connected with the influence of external currents on the properties of inhomogeneous regions were studied. The first works in this area were performed in one-dimensional or two-dimensional axisymmetric formulations.

As the computing power grew, the inclusion of gravity, the influence of magnetic fields was taken into account. In the papers [5] - [7] the problem of interaction of shock waves with a single MC was studied. The influence of the basic hydrodynamic characteristics and magnetic fields was investigated. One-dimensional and two-dimensional approaches are characterized by limitations that do not allow a detailed study of the interaction of the shock wave with the MC. In 3D case such limitations are absent. This gives additional advantages associated with a more correct description of emerging processes. In papers [8] - [9] two and three-dimensional approaches of the problem were used. In these and several other studies, it became possible to clarify complex interactions that arise in the interaction of strong shock waves with molecular dust clouds. The appearance of the Rayleigh-Taylor instability, the ablation processes in the formation of a turbulent flow and the radiation cooling of a cloud substance are studied.

In the paper [10] a single-phase gas model was used that reflects reasonably correctly the physical picture of the current. In the calculations it was assumed that the unperturbed matter of the ISM consists of a relatively warm matter ($\sim 10^4 K$) and small inhomogeneously distributed cold clouds ($\sim 10^2 K$), which have a high density [5], [8], [11]. Initially, the clouds are in dynamic equilibrium with the background gas [10].

In the paper, the simulation is carried out using high-resolution difference schemes, on sufficiently detailed grids. The processes of formation, evolution and interaction among themselves of filament structures, the appearance of supersonic turbulence, etc. are considered. Further gravitational contraction of the proto cores can initiate star formation processes.

2. Formulation of the problem

The interstellar medium consists of a relatively warm substance $\sim 10^4 K$. There are molecular clouds in the ISM, which density is much higher than the average ISM density. The temperature in the molecular cloud is less than the ISM temperature $T_{\text{cloud}} \sim 10^2 K$. We consider the problem of collision of two molecular clouds. The geometry of the computational domain is represented at Fig.2. A cross-section of the three-dimensional computational domain is shown by a plane perpendicular to the $z$ axis. The mentioned above cross-sections show the initial density distribution in the clouds.
Computer simulation of astrophysical problems as a rule requires a careful choice of applied numerical methods of high accuracy order and dimension of the computational grid. It is shown in the paper [6] that if numerical cell size is taking smaller than the local Jeans length \( \lambda_J \), nonphysical artificial fragmentation can arise in the calculations.

\[
\lambda_J = \left( \frac{\pi C_s^2}{G \rho} \right)^{0.5}
\]

To prevent such effects, leading to incorrect results, it is necessary to use refinement computational grids. The analysis showed that the minimum mesh size at which numerical Jeans instability disappears is equal \( 512 \times 512 \times 512 \) nodes. To avoid the occurrence of local Jeans instability high resolution grids (up to \( 2048 \times 1024 \times 1024 \)) were used in our work.

The computing area is a parallelepiped with dimensions from \( 2048 \times 1024 \times 1024 \) to \( 1024 \times 512 \times 512 \) cells along the \( x, y \) and \( z \) axes correspondingly. In our simulations the cell sizes along all axes \( \Delta x, \Delta y, \Delta z \) was the same: \( \Delta x = \Delta y = \Delta z \). The matter of the ISM and MC has its own sound speed, equal to \( a_i = \sqrt{\gamma_i \rho_i} \), \( i = 0, 1 \), (where \( i = 0 \) for ISM, \( i = 1 \) for MC) [12].

The Mach number for the ISM and MC we denote as \( M_i = u_i/a_i \). Following the paper [13, 14] we used the same adiabatic index \( \gamma = 5/3 \) for the whole computational domain. We neglect viscosity and consider nonstationary flows of compressible ideal gas. The system of conservation laws (mass, momentum and energy) in 3D Cartesian coordinates can be written in the following way:

\[
\frac{\partial U}{\partial t} + \frac{\partial \mathbf{F}(U)}{\partial x} + \frac{\partial \mathbf{G}(U)}{\partial y} + \frac{\partial \mathbf{H}(U)}{\partial x} = 0
\]

The vector of conservative variables can be written in the form: \( U = (\rho, \rho u, \rho v, \rho w, \rho e)^T \). The vector of fluxes is:

\[
\mathbf{F}(U) = \begin{pmatrix}
\rho u \\
\rho u^2 + p \\
\rho uv \\
\rho uw \\
\rho ve + up
\end{pmatrix}
\]

The fluxes \( \mathbf{G}(U) \) and \( \mathbf{H}(U) \) can be written similarly to (3). The equation of state we use in the form:

\[
p = \rho (\gamma - 1) \left[ e - \frac{1}{2} (u^2 + v^2 + w^2) \right],
\]

here \( \gamma \) is adiabatic index, \( \rho \) density, \( \mathbf{v} = \{u, v, w\} \) velocity vector and \( p \) pressure [12].
Initially, the cloud is in dynamic equilibrium with the background gas. Thermal conductivity and radiation losses during interaction can be neglected. The equation of state of an ideal gas with $\gamma = 5/3$ is used in this paper.

The ISM density is $\rho_a = 2.15 \times 10^{-25} \text{ g/sm}^3$, the temperature $T_a = 10^4 \text{K}$, the velocity $u_a = 0.0$. The cloud density is $\rho_c = 1.075 \times 10^{-22} \text{ g/sm}^3$, the temperature $T_c = 100 \text{K}$, $u_c = 0.0$.

One of the most important parameters of the process of shock-wave interaction with MC is the ratio of the density of MC to the density of ISM:

$$\chi = \frac{\rho_{mc}}{\rho_{ism}}$$

Here $\rho_{mc}$ – is the density of the molecular cloud, $\rho_{ism}$ – the density of the ISM.

Initial density distribution for our simulations was taken from [15], [16]. The density radial distribution formulas for clouds $C_1$ and $C_2$ are the following:

$$\rho(r) = \rho_{ism} + \frac{\rho_{cl} - \rho_{ism}}{1 + (r/R_{cl})^{2.7128}},$$

$$\rho(r) = \rho_{ism}(\chi + \frac{\alpha}{\alpha + 1}(1 - \chi)),$$

where $\chi = \frac{\rho_{cl}}{\rho_{ism}}$ – density contrast.

Form factor $\alpha$ in (7) can be calculated by formula:

$$\alpha = \exp\{\min[20.0, 10 \cdot ((\frac{r}{R_{cl}})^2 - 1)]\}.$$  

3. Numerical method

The solution of the equations (2 - 5) on the Euler grid uses the adaptive solver Roe, in which numerical fluxes are defined on all faces of computational cells. It is a modification of Godunov’s method [17], [18], [19] For the construction of an efficient parallel numerical algorithm and software complex, the spatial splitting method is used. The system of governing equations is written in operator form along the axes $x$, $y$, $z$. Thus, we can perform calculations for each coordinate independently. The parallelization with respect to spatial variables is organized.

To overcome Galilean’s non-invariance, one more step is taken in time, but the operators are executed in the reverse order. This is done to create a completely symmetrical three-dimensional calculation. Finally, we move from the time step $n$ to the step $n + 6$. For every operator, a scheme is used which is based on the Godunov method of high accuracy order.

The flux along one of the axes for the cell $j$ can be written in the following form:

$$Q_j^{n+1} = Q_j^n - \frac{\Delta t}{\Delta x}(F_{j+1/2}^{n+1} - F_{j-1/2}^{n+1}) + \Delta t S_j^{n+1/2}$$

Here $j$ is the cell center, $j \pm 1/2$ - relates to the cell boundaries. To calculate the state vector at a new time level, we need to know the flux vector with a half time index, as well as the left and right cell borders, and the $S$ vector in the cell at the half time step. The Courant-Friedrichs-Levy stability factor varied from $0.2 \leq CFL \leq 0.7$.

4. Parallel algorithm

The creation of parallel algorithms devoted to the solution of complex astrophysical problems allows one to study the dynamic evolution of the interstellar medium (ISM), MC, and the formation of new stars. Conducting numerical experiments in a three-dimensional setting on
Figure 3. Analyzing the quality of the parallelization of the program, performed with the Amplifier XE program

sufficiently detailed grids requires large computational resources. To perform the calculations, a parallel algorithm was developed for solving the problems of nonstationary gas dynamics [22].

The work uses an algorithm and a code that allows using multiprocessor computers for calculations. The program used OpenMP and CUDA technologies. The OpenMP was configured using Intel VTune Amplifier XE. This tool allows one to perform application profiling directly on the cluster node. The LightWeight Hotspots analysis type was used.

At the Fig. 3 are the results of the analysis performed on the parallelization of the program on the central processor. This figure shows the "quality" of the constructed parallel algorithm. More than 80% of the total time is occupied by the calculation of three subroutines. After optimization of these subroutines, their degree of parallelization has become quite high. At the figure, green color shows "ideal" parallelization, yellow - good, red - bad. Poor parallelization means that the efficiency in this case is less than 50%. Some subroutines were calculated on a graphics processor.

The results of calculations showed that for not very large grid sizes (up to 1024x512x512) parallelization on the GPU gave more acceleration than parallelization with OpenMP. With the increase in the size of the grid, the data can not be stored in the GPU memory.

5. Adaptive Mesh Refinement
In the calculated domain, regions with large gradients of temperature, pressure, density, etc. appear. These regions are neighbouring with regions of smooth behavior of the unknown functions. To increase the spacial resolution and reduce computational costs, in the regions of large gradients a more detailed grid with smaller cell sizes was created. This approach is called the Adaptive Mesh Refinement [20, 21]. The application of the Euler cubic grid in 3D provides a high interpolation order and does not require an additional adjustment of the initial grid topology.

The algorithm for constructing grids is implemented as follows. An initial coarse grid is defined. The density was chosen as the criterion for the subdivision. The lowest, coarse level is the original grid. Further subdivision into sublevels with a finer grids is realized as follows. Depending on the refining criterion, in each of the required areas, each cell is divided into eight
cells. If the splitting criterion is satisfied, the process of decreasing the size of the cells continues. The total number of nested subgrid levels depends on the physical problem and the specified split criteria. In Fig. 4 is an example of constructing such a grid.

![Figure 4. An example of adaptive grid construction.](image)

6. Results
The results of the simulation of two MCs central collision at speeds from 0.5 to 10 km/s are given. Under such conditions, a significant fragmentation of the clouds is observed, the gas is dispersed from the center to the periphery, and dense regions are formed in the collision region. Depending on the initial density and collision velocity, regions of increased density appear and increase in the contact zone, which can become gravitationally bound objects at later time. In Fig. 5 the results of calculations of the collision of molecular clouds at a mutual velocity of 5 km/s is represented. The dimensionless time moments are shown, in which smaller MC was inserted into a larger one by about the half the radius of a smaller cloud (right fragment). The center shows the contact area, which rapidly changes its shape and mass.

![Figure 5. The central collision of two MC. Left - formation of the contact area. In the center is the contact area and the velocity vector field. On the right, filament formation at a later time moment.](image)

Density contrast diagram, shown on Fig. 6 indicates a spatial intermittency of supersonic flow, accompanied by the amplified Kelvin – Helmholtz and and Richtmeyer – Meshkov instabilities.
and disturbance of gas at outer boundaries of the clouds [22]. During cloud deformation dense lens-like clumps and rolled rings arise here.

This process is represented in more detail in Fig.6. The time evolution of the field of a rapidly varying density contrast in the core (red color) and in the envelope (green color) is given. The maximum contrast of the density $\chi$, when collided at relatively low speeds, increases by two orders of magnitude, compared with the initial contrast $\chi = 500$. The change in the density, shape, and position of the contact surface leads to the appearance of oscillations that appear on the midlines (equators) of the MCs and the appearance of oscillations in the interstellar medium. With further interaction of the MCs, a shock-compressed, lens-like layer forms superdense regions (clumps), from which ring sound waves propagate outwards [23].

![Figure 6](image_url)

**Figure 6.** Time evolution of the density contrast in the core and in the envelope.

![Figure 7](image_url)

**Figure 7.** The density distribution in the collision of two MCs (left), The successive stages of the collision process (from the bottom to the top)(right).

At the Fig. 7 are the graphs of the density distribution at various stages of the collision (on the left). In the center, the density distribution in the lens-like contact region is given. Right part of the figure - the destruction of the MCs shells and the formation of filaments at successive time moments.
7. Conclusions
The process of filament formation, superdense, gravitationally bound objects and destruction of molecular clouds is studied. A mathematical model is constructed and computer simulation of this problem is carried out on multiprocessor systems using graphic processors. The morphology of the formation of the instabilities of Kelvin-Helmholtz and Richtmeyer-Meshkov has been studied.

It was shown that mutual collisions of molecular clouds cause supersonic turbulence, which could lead to oscillations, filament formation and superdense regions (clumps), and to the formation of gravitationally bound regions and the possible appearance of new stars.

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