Computational Modeling of Turbulent Structuring of Molecular Clouds Based on High Resolution Calculating Schemes

Boris Rybakin[1]✉, Valery Goryachev[2], Stepan Ageev[1]

[1] Department of Gas and Wave Dynamics, Moscow State University, Moscow, Russia
rybakin@vip.niisi.ru
[2] Department of Mathematics, Tver State Technical University, Tver, Russia
gdv.vdg@yandex.ru

Abstract. The article submits the results of 3D computational modeling of the adiabatic interaction between a shock wave and molecular clouds, central impact and glancing collision between them, in the case of counter movement. According to the problem set in the first case, two spherical clouds with pre-established density fields interact with the post-shock medium of supernova blast remnants. It is demonstrated that the collision give rise to the supersonic turbulence in a cloud mixing zone, the formation of cone-like filamentous structures, the significant stratification of gas density and the disruption of clouds. Problems of vortex filaments origination in clouds wakes are analyzed after simulation of supersonic forward and glancing collision of two molecular clouds.

Keywords: Parallel Computing · Supersonic Turbulence · Shock Waves · Small Molecular Clouds.

1 Introduction

Giant molecular clouds (GMC) are a huge accumulation of interstellar gas and dust, composed mostly of molecular hydrogen. They are the coolest and densest portions of the interstellar medium (ISM). MCs are generated from this matter, a part of which falls under strong shock wave compression in extended filaments and globules that eventually collapse. Filaments formations are wide spread in the universe. Swellings of filaments and clumps occurring inside MCs are results of shock strong compression and cloud's self-gravitation, magnetic hydrodynamics after-effect [1, 2]. Molecular clouds may evolve to structure of interlacing and connecting filaments. This web of spatial voids, highly compressed gas fibers or enclosures, depends on the external influence on the interstellar medium, and has an indirect action on the condensation of cores formed into more massive intersected filament clumps that later could become protocores – embryos of future stars [3, 4].

One of possible scenarios of filament structuring initiation is a collision of MCs with strong shock waves (SW) of another gas formations propagated in the space. Others cases are initiated in different collisions between MCs of different mass with originating shock wave multiformity in mixing zones.

The shock wave interaction generated by proliferation of supernova explosion remnants and the molecular clouds leads to supersonic turbulence of gas in MCs, deep density stratification and their destruction followed by formation of filamentous structures. The shock wave impact accompanied by intense dynamic interaction of filaments with each other leads to the significant redistribution of gas density in MCs.

The present simulation has been performed to study vortex structuring in the molecular clouds formations disbalanced after collisions with a strong shock wave and between two MCs in different cases of collision, and associated with turbulization and filaments formation during these processes. The occurring filament formations governed by the vortex slipstream flow after MCs and a shock wave interact with each other and develop in the gradient regions of the gas density fields. It is shown that at specified points of time there occur ultra-dense regions, with the density contrast being an order of magnitude higher than the initial contrast in clouds. Evolution of such objects, running from the formation of filament rudiments to the moment, they reach the stellar densities, covers a vast range of spatial and time scales.

Main of numerical methods used in astrophysical hydrodynamics can be divided into classical continuum approach and Smoothed Particle Hydrodynamics (SPH) methods. A significant part of continuum solvers uses a high resolution regular or AMR grids. The most of them work on parallel HPC. SPH methods are challenges due to several benefits over traditional grid-based techniques (flexible parallel computing realization, multiphase fluid simulation, etc.). This method, however, has essential limitation, for example, particles leaved a domain with high gradient parameters (velocity, pressure) will be compensated, and this leads to loss of computational accuracy. Recent related publications using last approach can be found in [5-9].

Author's code used is a continual. The article submits the results of 3D computational modeling of the adiabatic interaction between a shock wave and molecular clouds, central impact and glancing collision between them. The article analyses the density fragmentation, investigates the process of filament formation and gas density stratification as a result of SW/MCs or MC/MC collision. Applying HPC technologies we have realized a numerical simulation of complicated gas dynamics task using calculation grids with more than two billion nodes.

2 Problem definition

2.1 Initial conditions and parameters

We study three scenarios of MCs collision in ISM. Case I: strong shock wave and SW/MCs interaction in a configuration where a plane of shock frontal of supernova remnant gas runs onto systems of two clouds of spherical form. Case II: a central concussion of two molecular clouds (MC/MC) of initially spherical form moving in opposite direction. Case III: a glancing collision of MC to the side of another one, in reverse moving.

The schema of simulated collisions is shown in Figure 1. Two MCs have different radial distribution of density (illustrated by different diagrams on schema).

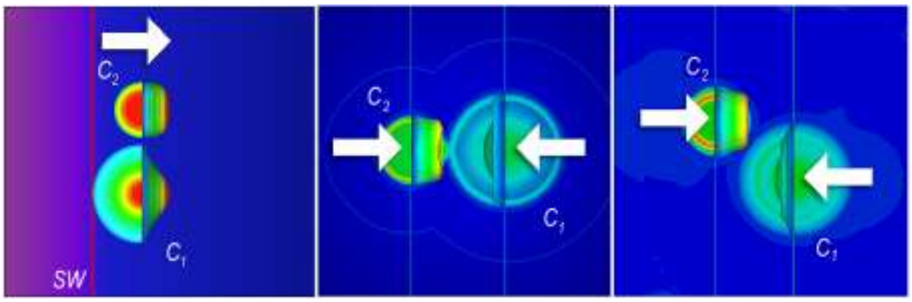

Fig. 1. Computation schemes for three case of simulation.

In the case I, at the moment of collision a shock wave contacts with outer MCs boundaries. Special rule of density radial distribution is used to represent more realistically the density smoothing profile on the border between the clouds and the outer medium. Appropriate functions were taken according to recommendations given in [10-12].

The density radial distribution formulas for clouds C_1 and C_2 are the following:

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

$$\rho(r) = \rho_{ism}\left(\chi + \frac{\alpha}{\alpha + 1}(1 - \chi)\right) \quad (2)$$

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

Form factor α in (2) can be calculated by formula

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

Several parameters in these formulas controlling the steepness of clouds border were changed to improve density smoothing.

The key physical parameters and assumptions of the present tasks were correlated by data from [17]. The interstellar medium consists of relatively warm matter with $T_{ism}=10^4$ K, the temperature of colder MC gas $T_{cl}=10^2$ K. The ambient gas density of the outer cloud medium $\rho_{ism}=2.15\times10^{-25}$ g·cm^{-3}, the gas density in the undisturbed cloud centers $\rho_{cl}=1.075\times10^{-22}$ g·cm^{-3}.

In the case I, characteristic (conventionally diffused) radius of each cloud R_{cl} is equal roughly to 0.1 pc. For system of two clouds (C_1, C_2), the mass of each is (approximately, considering fuzzy boundary) equal to $0.005M_\odot$ or $0.01M_\odot$ respectively, in solar mass fractions. The initial density contrast between the MCs centers and the interstellar medium is $\chi = 500$.

Mach number M_{sw} of incident shock wave is equal to seven, post-shock plasma density $\rho_{sw} = 8.6\times10^{-25}$ g·cm^{-3}, temperature $T_{sw} = 1.5\times10^5$ K, velocity of shock wave $U_{sw} = 104$ km·s^{-1}. The thickness of post-shock wave front is ~ 2 - 5 pc, which is much greater than the radius of a cloud. The period of time the shock wave propagates the upper cloud diameter is about 2000 years. This value is used as a scale for non-dimensional time.

In the case II, III the mass of each cloud C_1, C_2 is equal to 0.32 $M_\odot$ or 1.05 $M_\odot$ respectively. The velocity of each MC is 5 km·s^{-1}, the oncoming velocity is equal 10 km·s^{-1}. In the case of the glancing strike centers of MCs are displaced, linear shift is $0.2R_{cl}$. The initial density contrast between the MCs centers and the interstellar medium is $\chi = 500$ and 100 accordingly.

2.2 Equations and numerical realization

Gas movement is described with a set of Euler equations which are conservation laws for mass, momentum, and energy

$$\frac{\partial U}{\partial t} + \nabla \cdot T = 0\,,\ U = \begin{pmatrix} \rho \\ \rho \boldsymbol{u} \\ e \end{pmatrix},\ T = \begin{pmatrix} \rho \boldsymbol{u} \\ \rho \boldsymbol{u}\boldsymbol{u} + pI \\ (e+p)\boldsymbol{u} \end{pmatrix}^T,\ e = \frac{p}{\gamma - 1} + \frac{|\boldsymbol{u}|^2}{2}\,, \qquad (3)$$

ρ denote the gas density, $\mathbf{u} = (u, v, w)$ is the velocity vector. The total energy density e and gas pressure p are related through the ideal gas closure, where adiabatic index - $\gamma = c_p/c_v$ is equal to 5/3.

Accuracy of numerical solution of multivariable problems in supersonic gas dynamics is eminently important in astrophysics phenomenon simulation. High-order accurate difference schemes have guaranteed monotonicity preservation of conservation laws. They are based on Godunov approach [18] to proof linear, first-order upwind schemes. The nonlinear, second-order accurate total variation diminishing (TVD) approach provides high resolution capturing of shocks and prevents unphysical oscillations, therefore it describes the local discontinuity preserving hyperbolic conservation laws [19,20]. The TVD maintains a nonlinear stability condition. The total variation of a discrete solution defined as a measure of the overall amount oscillation in velocity **u** is

$$TV(u^t) = 2\left(\sum u_{max} - \sum u_{min}\right). \qquad (4)$$

The flux assignment scheme with condition $TV\left(u^{t+\Delta t}\right) \le TV\left(u^t\right)$ can guarantee that the amount of total oscillations will have a limit. Different TVD limiters are used: *minmod*, *superbee*, *vanleer*. The *vanleer* limiter proves to be preferential in our solution. TVD scheme is an approbated and robust method to solve systems of Euler equations. Such an approach and a sampling of physical coordinates [22] have enables us to take an appropriate parallelization and accelerate computing.

Numerical experiment is performed using different spatial resolution of physical description of SW/MCs collision in space. Grid sizes from 512×512×512 (case II and

III) to 2048×1024×1024 (case I) units were used in systematic calculations. Minimal spherical clouds radius corresponds to 128 grid nodes. Last number exceeds the spatial resolution level, which is necessary to resolve correctly density and velocity turbulence fluctuations over energy high gradient gas layers and shock waves. The level of zonal discretization is more that used in [14-16]. The computing areas used for problem under consideration are parallelepipeds with dimensions 1.6×0.8×0.8 pc for the case using high resolution mesh, and 1.6×1.6×1.6 pc for MC/MC collisions. The lateral and outlet computational domain edges are determined as open boundary conditions for primitive variables.

We use author's parallel code allowing computations to be done with OpenMP. The setting of a code performance is done with Intel VTune Amplifier XE. Some computations are done with graphics accelerators NVIDIA K40 and CUDA for PGI Fortran. To compute with graphical accelerators the computation program has been retargeted so that some subprograms should be directed to GPU and the others - to CPU.

The numerical simulation procedure and peculiarities of 3D hydro code were detailed in [22, 23]. The wide set of CFD utilities and postprocessing systems were used to analyze a big data output after a numerical experiment. Simulated filamentous structures and fragmentation process observed are analyzed using computer visualization technique of author's program - HDVIS.

3 Analysis of SW/MCs and MC/MC collision

Numerical simulation has been performed to study the morphology and vortex coherent structures in the molecular cloud formations disbalanced after collisions with a shock wave, shift and wake reformation in the situation with MCs forward and glancing impact.

The computations have shown that the formation of filaments and gas density stratification depend significantly on several factors, but the primary one is a shock wave compression of clouds matter near the sheet (inners and outers) layers of gas mixed.

3.1 SW/MCs interaction

In first case of SW/MSs collision the density gas fragmentation is associated with supersonic turbulization during these processes. The evolution of transient coherent structures in MCs after passing a shock wave goes through three representative stages. At initial time, when a bow shock wave rounds clouds, a wave is formed behind its front. It moves towards the flow and forms vortical structures, as it is shown in Figure 2. Iso-surfaces of density contrast χ =10 and 2000 and twisting pathlines are given in green and red colors.

At the next stage a SW continues to extend and initiates the Richtmyer-Meshkov instability (RMI) - disturbance of gas at outer boundaries of clouds. There occur convective acceleration of flow and whirling of the boundary layers of the conventional border between MCs and a surrounding matter, in zones with large and small gas density. The Kelvin–Helmholtz instability (KHI) can increase here additionally.

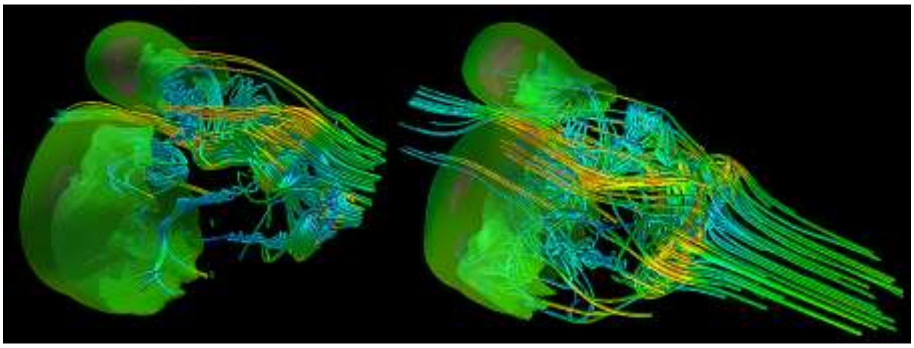

Fig. 2. Initial compression in SW/MCs interaction (t = 40, 60).

At the third stage of cloud transformation, the conical-like sheets commence to stretch. The flow streams accelerate in high gradient density layers and can initiate whirling of layers at the conventional MCs/ISM borders. Filament rudiments look like the elongated conical folded sheets (Figure 3, 4). The global circulation of a gas flow in the mixing zone begins to appear after cloud C_1 being rounded by a shock wave and finds its source in two vortex lines born inside the cloud at the back side. The flow swirl occurs in accordance with the scheme of spatial twin vortex.

Fig. 3. Gas density stratification and vortical structure of MCs at t = 330.

Vortex sheets start to deflect and twist and become filamented practically after origination of instability. The observable vortices are illustrated in Figure 3 by showing of vorticity magnitude $|\omega|=30$ distribution. In the evolution process, the vortex lines elongate, kink, take the form of hairpins, and expand in a bend region. The visualization inset shows the formation of a hairpin structure near the outer gas layer that precedes the long streaks. Transition happens via streaky and misshapen structures behind shock layers on the leeward side of MCs. Hairpin vortices observed are similar to those found in plasma flows for high Mach boundary layers in supersonic transition, investigated in experiment.

Q-criterion - the second invariant of a velocity gradient tensor being used to identify the regions of non-uniformly scaled vortex concentrations and to differentiate peculiarities of the flow structure. Vortices have smaller distribution density within the mixing region, at the boundaries and surfaces of elongated filamentous film rudiments the vortex distribution densities are significantly higher and show a local velocity slope in different cloud regions. Figure 3 shows typical vortex formation: with elongated loops and helical deformations inside MCs at the moment of shell forming.

To reinforce the role of density interleaving and turbulent supersonic transfer in analyzing of MCs stratification the denstrophy characterization is used. The local denstrophy is defined as a value: $\Omega_{1/2} = \frac{1}{2}\left| \nabla \times \left(\rho^{1/2}\boldsymbol{u}\right)\right|^2$, which is an indicator of compressible turbulent velocity fluctuation [24]. A view of iso-surface of denstrophy $\Omega_{1/2} = 1000$ at t = 300 is shown on Figure 4.

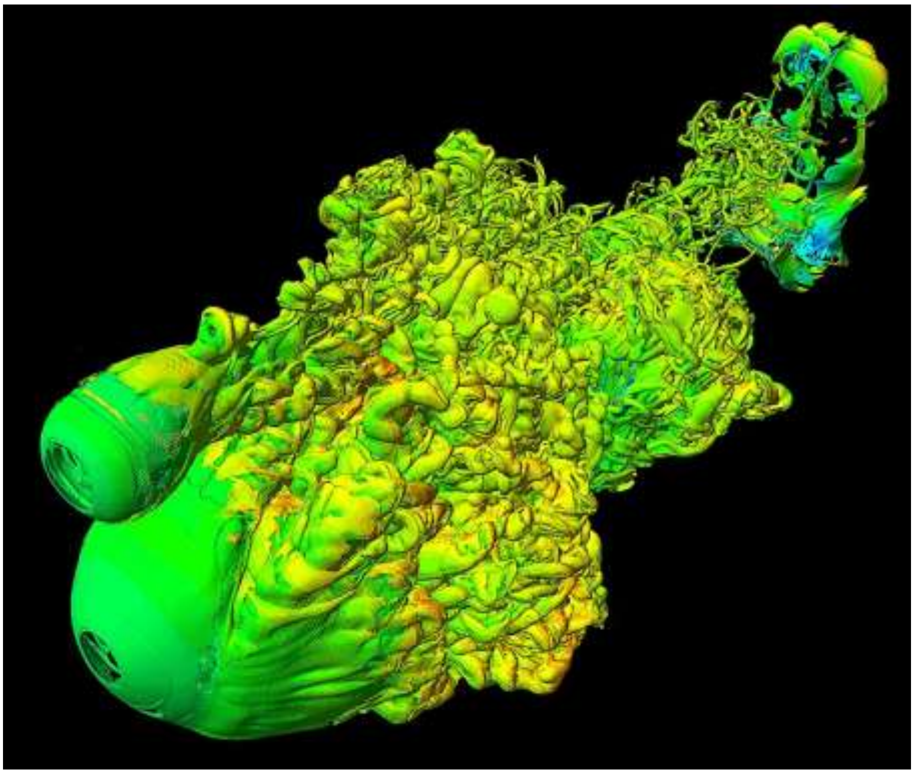

Fig. 4. Denstrophy distribution and vortex structure of MCs.

Scanning of denstrophy distribution iso-surface one can emphasize the fractal recurrence of cone-like filament envelopes. Supersonic flow perturbation leads to a considerable grow of the denstrophy over filament in stripping phase of MCs transformation. Compressed gas sheets assume funneled form. The low-density gas is removed to center zone of cloud, and occupy low-pressure regions previously created by rarefaction waves. Stochastic void swelling is typical for shock-induced MCs. Generated vortices grow over time, slip and roll through the newly-formed sheets, eventually to be expelled outside.

One of the extreme forms of gas stratification in MCs is conventionally hollow filament. Envelopes of such formation are shown in Figure 5 using selected display of iso-surfaces for contrast density χ = 1 (opaque red-green-yellow), 5 (translucent rose). The map of local denstrophy is distributed along the surface of χ=1. Denstrophy color legend conforms to $100 < \Omega_{1/2} < 10000$. One can see that separate zones are practically eddy-free; they have the close to ISM density of gas. Hollow channels and caverns with low denstrophy and turbulent pulsation are intrinsic for giant molecular clouds.

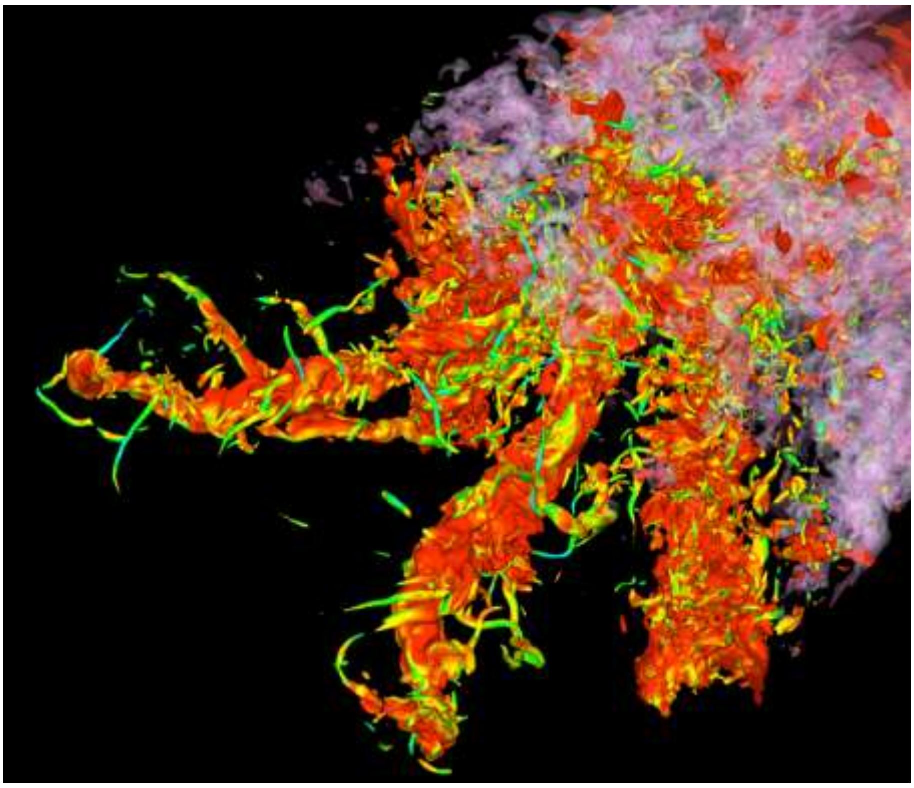

Fig. 5. Iso-surfaces χ=1, 5 with denstrophy contours at t=300.

Supersonic turbulence drives the fragmentation of dense cores and multiformity of pro-filamentary structures taking the original shell-like and clump forms. It is possible to establish some relationship between energy and density gradients strips on shell edges which is high-correlated. Gas currents near edges are accelerated by oblique collisions of secondary shock fronts that can arise from the initial supersonic shock fluctuations, either over the cloud recirculation zone or inside it, or behind the shock wave (primary or secondary) intersection lines and discs.

3.2 MC/MC collisions

Collision of SMCs or molecular clumps in GMC can be realized in different ways. Outcomes of impact depend on initial parameters: velocities, mass ratio, impulse direction, matter inhomogeneity and another thing. In our study results of central and shifted collision have been explored as first. The parameters and initial conditions for formulated tasks assigned in section 2.1.

Central impact between two molecular clouds studied with oncoming velocity of objects equal 10 km·s^{-1}. The mass ratio M_{c1}/M_{c2} in this collision is much less of three. Under such conditions the collision is accompanied by density fragmentation and gas scattering from the center to periphery outside. Time sequence of collision compressing is shown on Figure 6.

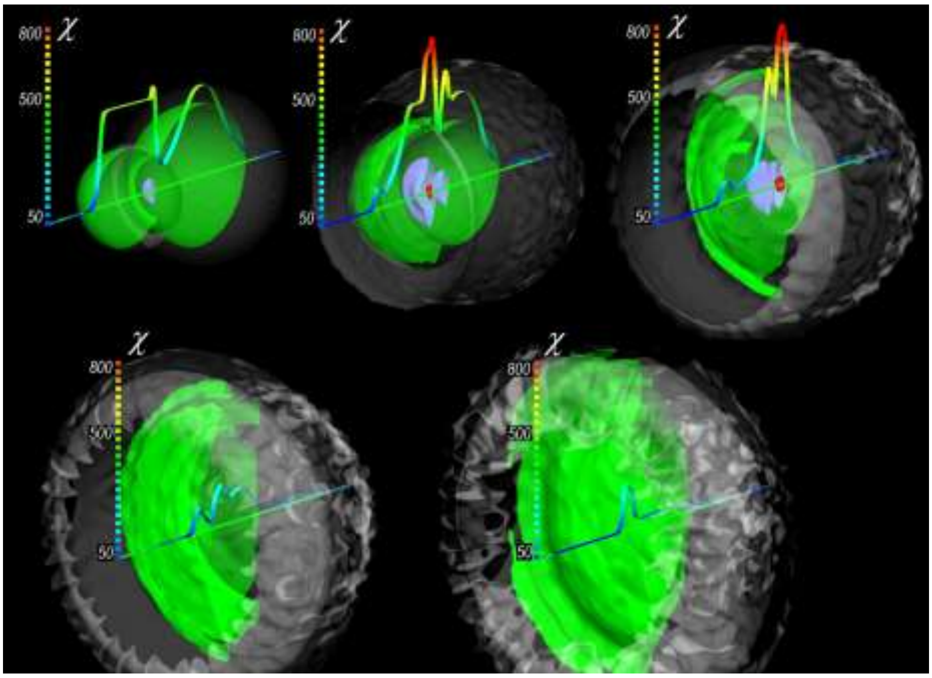

Fig. 6. Central impact of two MCs, time sequence t = 5, 10, 15, 20, 25. Iso-surfaces χ = 10, 50, 500, 800 and density contrast profile on the central line.

Arising from forward compression a density "splash" is similar to concave lens of asymmetrical form. Substance of cloud C_2, of smaller diameter having much larger mass penetrates into cloud C_1 – lightweight, of a greater diameter.

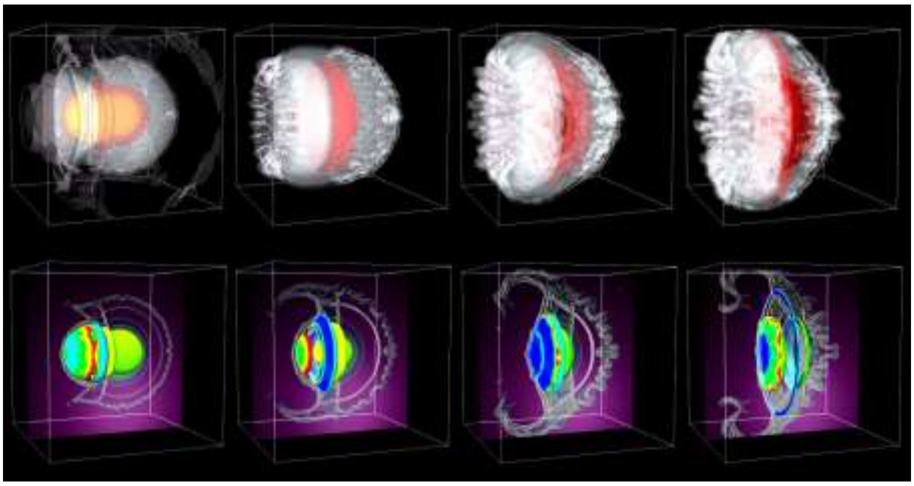

Fig. 7. Density contrast fields χ = 1, 5, 40, 100 in time evolution for central impact of MCs. Iso-surfaces of χ=100 and schlierens in the middle plane. Time sequence from t = 10 to t = 25.

Density contrast diagram, shown on Figure 6 indicates a fast (relatively to space time scale) spatial intermittency of supersonic flow, accompanied amplified KH instability and disturbance of gas at outer boundaries of clouds. During cloud deformation two-three compressed density lens-like clumps and rolled rings arise here (Figure 6, 7).

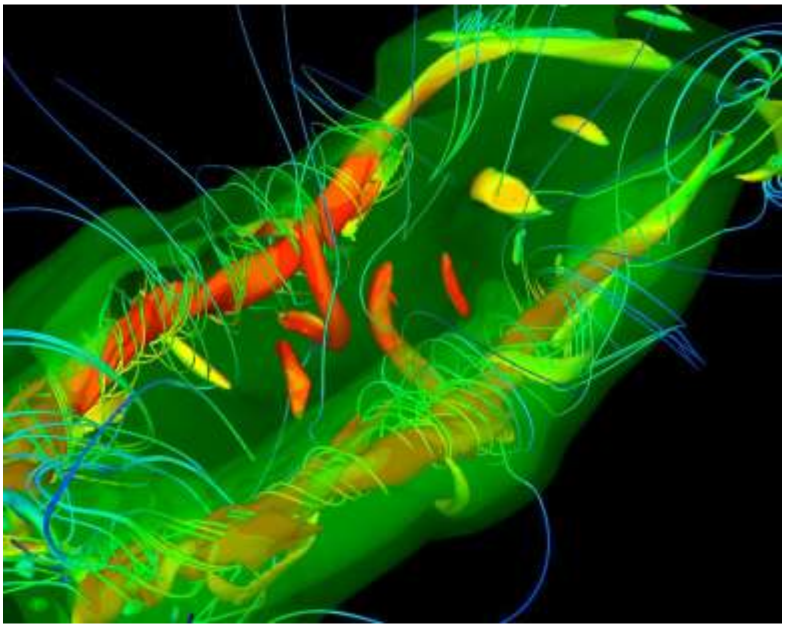

Fig. 8. Rolled filament layers of density contrast χ = 4, wake vortices, indicated by Q = 3, and helix pathlines for case of MC/MC glancing collision at time t =15.

The impulse does not lead to appearance of angular momentum. In work [7], using SPH modeling, a small rotation around central axis of clumps was discovered. Possibly it is due by mathematical setup to initial conditions in smooth particle approach and initial perturbation in solution.

The hot gas of colliding MCs is cooling rapidly. It can significantly affect the possible collapse of cool and heavily compressed protocores after collision. On figures given above one can see that from time moment t = 15 mutable density clumps began to break up leading to density fragmentation. Results of simulation are correlated well with observed data [11, 12].

In the case of glancing collision more heave molecular cloud penetrates into more light and friable side of another one. MC_2 cuts gas "hollow" in side of MC_1, boundary layers and conditional edges of which begin to roll. Time evolution of MCs separation process is shown in Figure 8, 9.

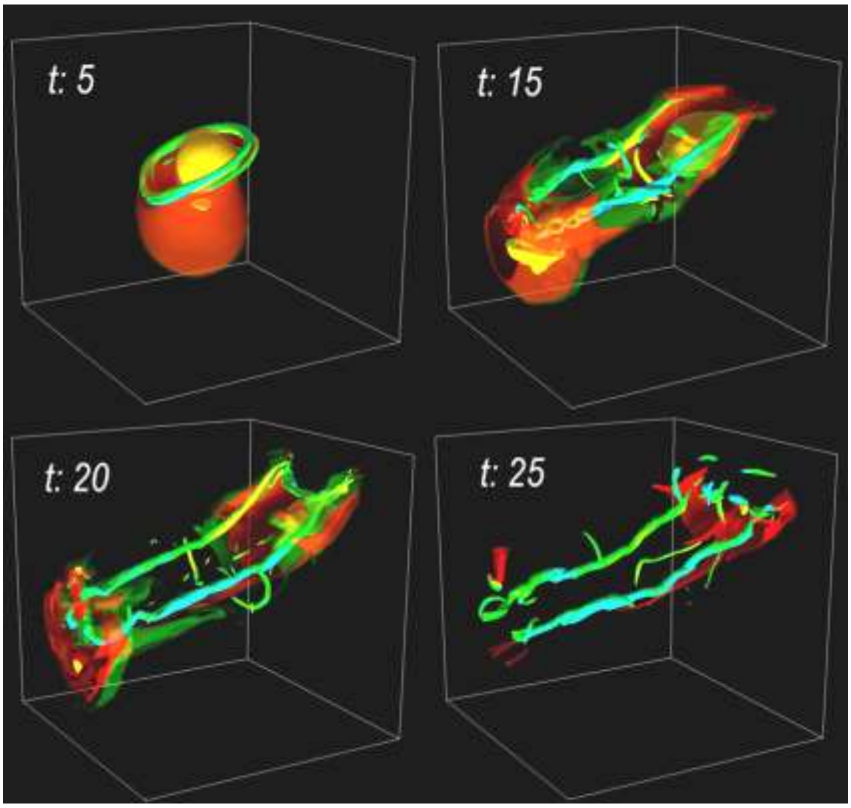

Fig. 9. Envelope layers of density contrast χ = 5, 10, 50 and vortex indicator Q = 5 for case of glancing collision of MCs. Origination of vortex tubes over filament sheet edges is shown.

Bound of mixing zone becomes film-like with curvilinear profile of their outer surfaces. Initially closed edges of cutting concavity become twisted and stretch. System of wake vortex tubes after simultaneous multidirectional passing of molecular clouds fairly stable on time scales examined in simulation.

Lens-like and cone-like clumps can be fragmented and ablated. Strong shock waves, dynamical supersonic collisions and local high compression zones shaking can be amplified by self-gravitation and MHD deformation of filaments originated in MCs.

The simulation SW/MCs/MC collisions taking into account self-gravitation process and magnetic condensation requires sharp increase of solution exposure, maybe even ten times over. To clarify possible developments of formed structures with more real time and spatial scales, it is necessary to carry out the numerical research using more power HPC systems.

Conclusions

1. Filaments forming and molecular clouds crushing were simulated using the HPC numerical modeling with high spatial resolution grids and parallelization codes developed.
2. The MCs dynamical transformation for different scenario of molecular clouds collision - between shock wave and MCs and impact between them - were analyzed in terms of supersonic perturbations over shocked sheets as the outcome of local strong shock compression.
3. The research has shown the ways the shock interaction initiates supersonic turbulence in mixed clouds, its effect on the filament origin and stratification of gas density, as well as on the transformation of emerging structures.

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