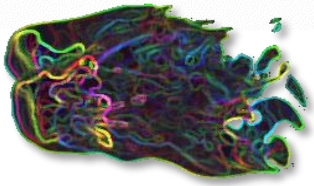
25-26 09 2017, Moscow

Russian Supercomputing Days

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



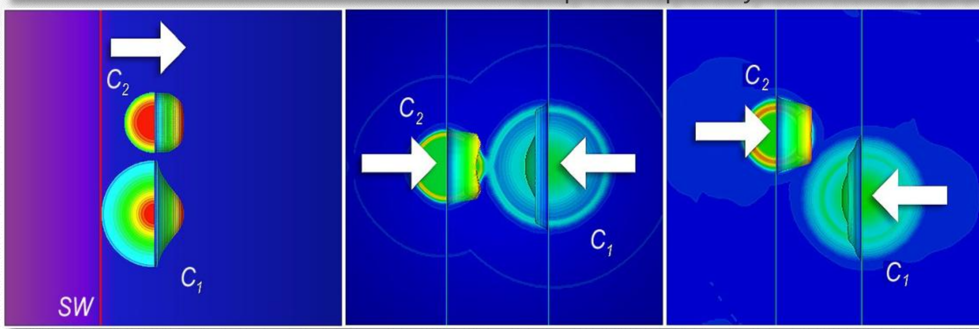
Boris Rybakin*, Valery Goryachev** and Stepan Ageev*

* SRISA RAS, Dep. of Gas and Wave Dynamics, MSU, ** Dep. of Mathematics, TvSTU

# MCs/SW (case I) and MC/MC (case II, III) collision

The present contribution is aimed at numerical modeling of supersonic turbulization of MCs initiated by:

1) strong shock wave from SNR blast oncoming on two molecular clouds
2) central impact and glancing collision of two MCs moving in opposite direction




It is a red super giant star in the constellation of Monoceros. Recently the star flared up bursting out with a bright light, like a nova. As the light travelled away from the star in all directions like ripples in a pond it encountered dust and gas in space periodically after leaving the star. The effect is called Light Echo.

Star V838 Monocerotis Light Echo

Photos were taken by the Hubble Space Telescope from early 2002 until 2006.

A molecular cloud is a large complex of interstellar gas and dust, composed mostly of molecular hydrogen but also containing many other types of interstellar molecule. MCs are the coolest (100 to 200 K) and densest ($10^{-20}$ to $10^{-22}$ g/cm$^3$) portions of the ISM. Stretching of Giant Molecular Clouds typically over several hundred light-years and containing million solar masses of material, they are the largest gravitationally-bound objects in the Universe. Molecular clouds are the only places where star formation is known to occur.

# Problem definition

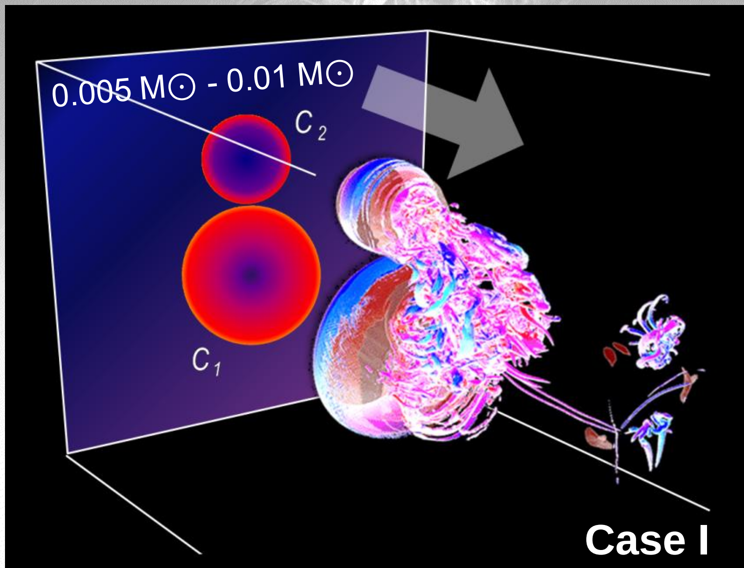
Gas movement generated by shock wave which runs onto molecular clouds system or MC/MC collision is described with a set of Euler equations which are conservation laws for mass, momentum, and energy.

$$\frac{\partial U}{\partial t} + \vec{\nabla}\cdot T = S \qquad U = \begin{pmatrix} \rho \\ \rho\bar{v} \\ e \end{pmatrix}, \quad T = \begin{pmatrix} \rho\bar{v} \\ \rho\bar{v}\bar{v} + pI \\ (e+p)\bar{v} \end{pmatrix}^{T} \qquad e = \frac{p}{\gamma - 1} + \frac{|\bar{v}|^{2}}{2}$$

The total energy density *e* and gas pressure *p* are related through the ideal gas closure.

where $\rho$ is the mass density, $\boldsymbol{u} = (u, v, w)$ 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.

# Initial setup for two cloud system MCs/SW




$$\rho(r) = \rho_{ism} + \frac{\rho_{cl\bullet} - \rho_{ism}}{1+\left(\frac{r}{R_{cl}}\right)^{2.718}}$$

Johansson, E. & Ziegler, U. 2011.

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

Pittard, J.M. at al. 2009.

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

Density contrast

$$\chi = \frac{\rho_{cl\bullet}}{\rho_{ism}}$$

Molecular clouds : $R_{cl}$= 0.1 pc (resolution of $C_2$ is 128 grid nodes) $T_{cl}$ = 100 K, $\rho_{cl}=1.075\times10^{-22}$ g sm$^{-3}$

Density $\rho_{ism}= 2.15\times10^{-25}$ g sm$^{-3}$ Ambient temperature of the interstellar medium $T_{ism} = 10^4$ K

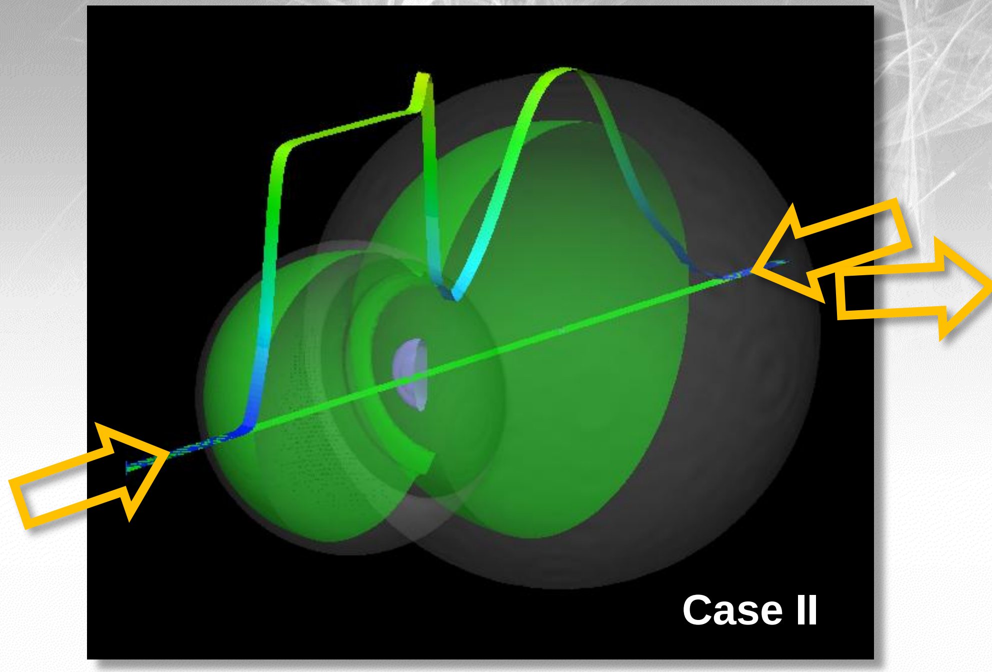
Initially $\chi = \rho_{cl\bullet} / \rho_{ism} = 500$. M = 7, $u_{sh}$= 104 km/s, $\rho_{sh}= 8.6\times10^{-25}$ g sm$^{-3}$, $T_{sh}= 1.5\times10^5$ K

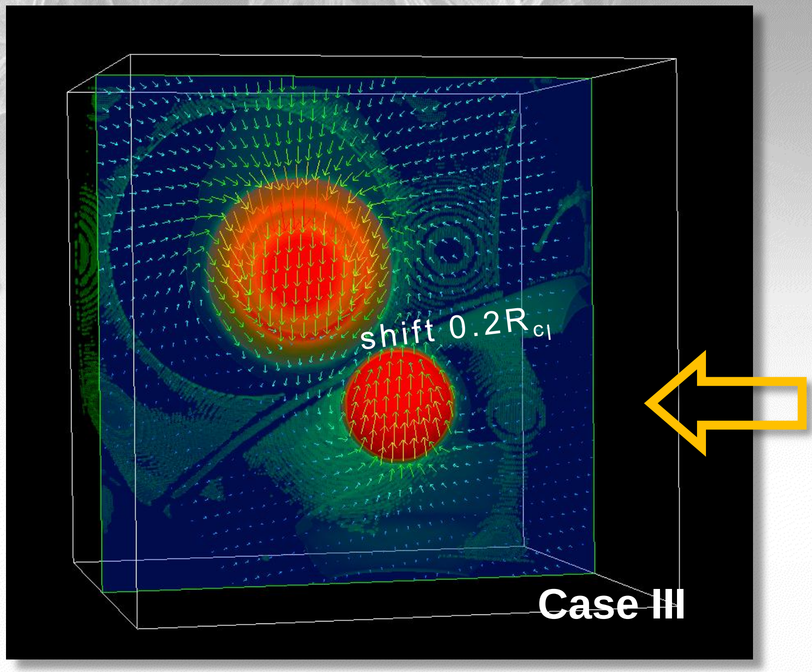
Post-shock wave front thickness ~ 2-5 pc

Grid X×Y×Z - nodes : 2048×1024×1024

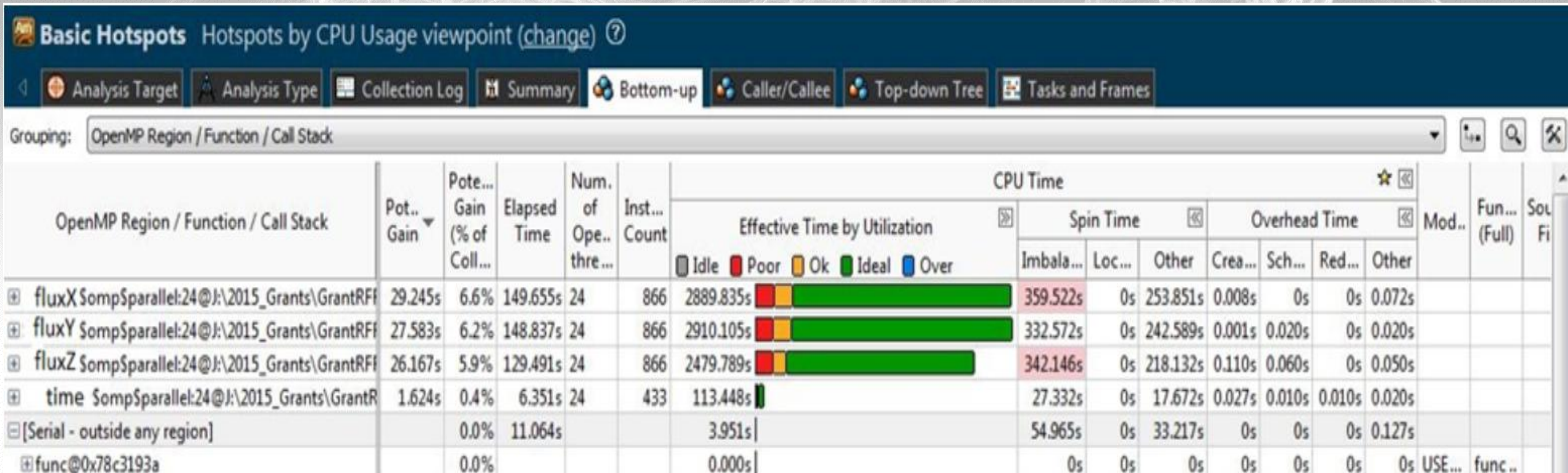
The time of passage of the shock wave over clouds $t_{swoc}$ : 2000 years

# Initial setup for central impact (case II) and glancing (case III) MC/MC collision




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 $0.2R_{c1}$.
The initial density contrast between the MCs centers and the interstellar medium is $\chi$ = 500 and 100 accordingly.



Basic Hotspots Hotspots by CPU Usage viewpoint (change)

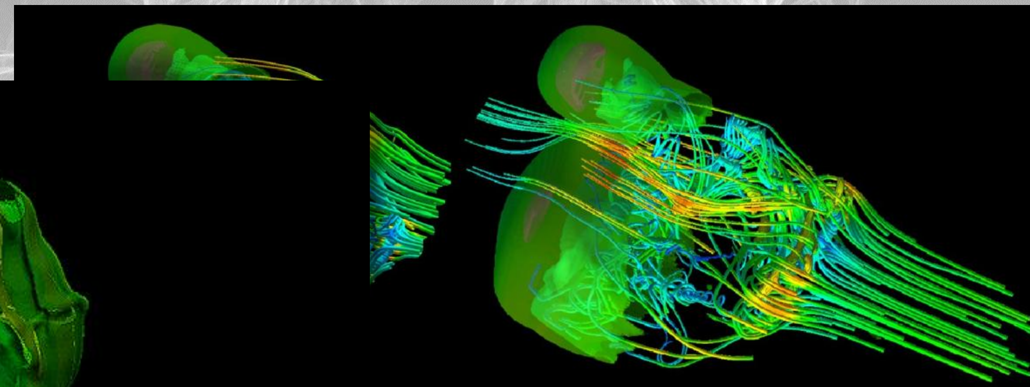
Analysis Target | Analysis Type | Collection Log | Summary | Bottom-up | Caller/Callee | Top-down Tree | Tasks and Frames

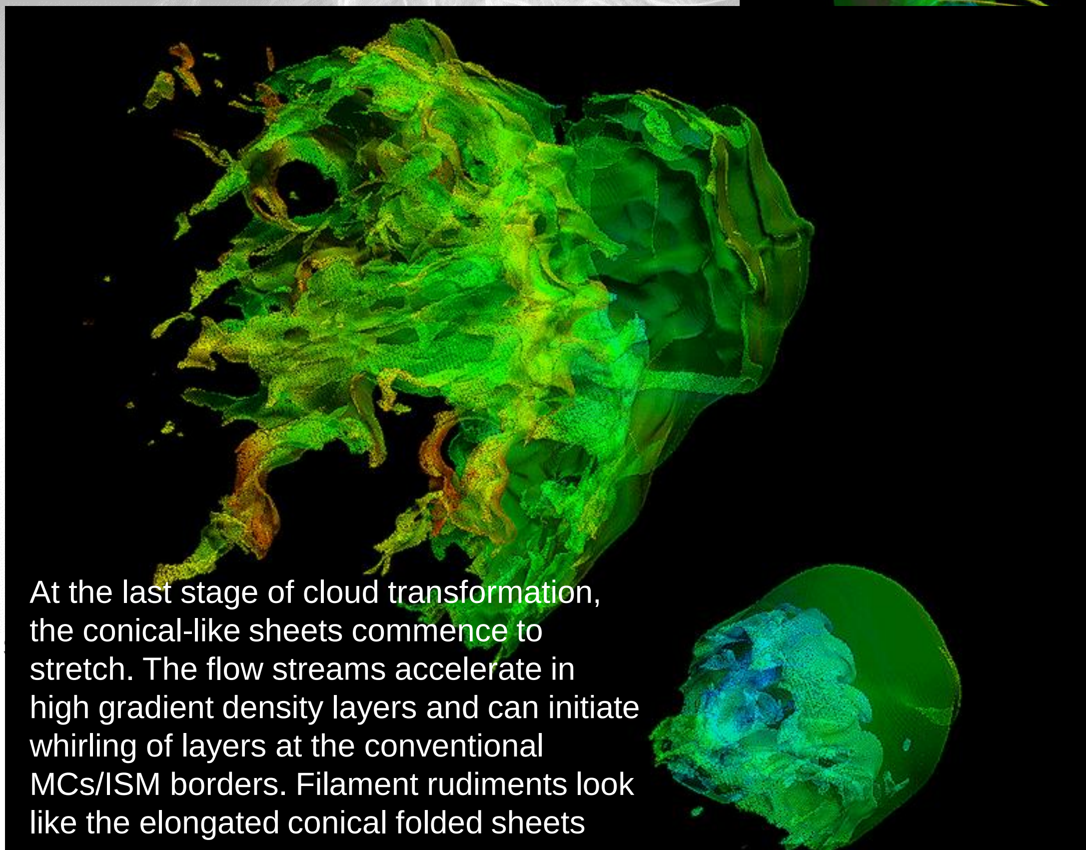
Grouping: OpenMP Region / Function / Call Stack

| OpenMP Region / Function / Call Stack | Pot.. Gain | Pote... Gain (% of Coll... | Elapsed Time | Num. of Ope.. thre... | Inst... Count | CPU Time: Effective Time by Utilization (Idle, Poor, Ok, Ideal, Over) | CPU Time: Spin Time: Imbala... | CPU Time: Spin Time: Loc... | CPU Time: Spin Time: Other | CPU Time: Overhead Time: Crea... | CPU Time: Overhead Time: Sch... | CPU Time: Overhead Time: Red... | CPU Time: Overhead Time: Other | Mod.. | Fun... (Full) | Sou Fi |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| fluxX $omp$parallel:24@J:\2015_Grants\GrantRFf | 29.245s | 6.6% | 149.655s | 24 | 866 | 2889.835s | 359.522s | 0s | 253.851s | 0.008s | 0s | 0s | 0.072s | | | |
| fluxY $omp$parallel:24@J:\2015_Grants\GrantRFf | 27.583s | 6.2% | 148.837s | 24 | 866 | 2910.105s | 332.572s | 0s | 242.589s | 0.001s | 0.020s | 0s | 0.020s | | | |
| fluxZ $omp$parallel:24@J:\2015_Grants\GrantRFf | 26.167s | 5.9% | 129.491s | 24 | 866 | 2479.789s | 342.146s | 0s | 218.132s | 0.110s | 0.060s | 0s | 0.050s | | | |
| time $omp$parallel:24@J:\2015_Grants\GrantR | 1.624s | 0.4% | 6.351s | 24 | 433 | 113.448s | 27.332s | 0s | 17.672s | 0.027s | 0.010s | 0.010s | 0.020s | | | |
| [Serial - outside any region] | | 0.0% | 11.064s | | | 3.951s | 54.965s | 0s | 33.217s | 0s | 0s | 0s | 0.127s | | | |
| func@0x78c3193a | | 0.0% | | | | 0.000s | 0s | 0s | 0s | 0s | 0s | 0s | 0s | USE... | func.. | |

Presented computations were conducted on two 12 cores (HT) of the Intel Xeon E2680 processor and on one, two and four graphic accelerators on each unit. Intel Vtune Amplifier XE was used to profile the code using CPU. Operating quality of in-house code is perfectly tolerable. The computation of three sub-procedures has 80% of CPU time. After optimization a parallelization possibilities of mentioned subroutines become sufficiently more high. To calculate fine details we used grids with resolution to 2048×1024×1024 units. We have used author’s 3D computer code, being controlled using OpenMP and proved by tasks being to those under consideration. High resolution numerical grids (more than two billion nodes) were used in parallel calculations on multiprocessor hybrid computers.

# Case I: stretch and conical-like sheet deformation of MCs

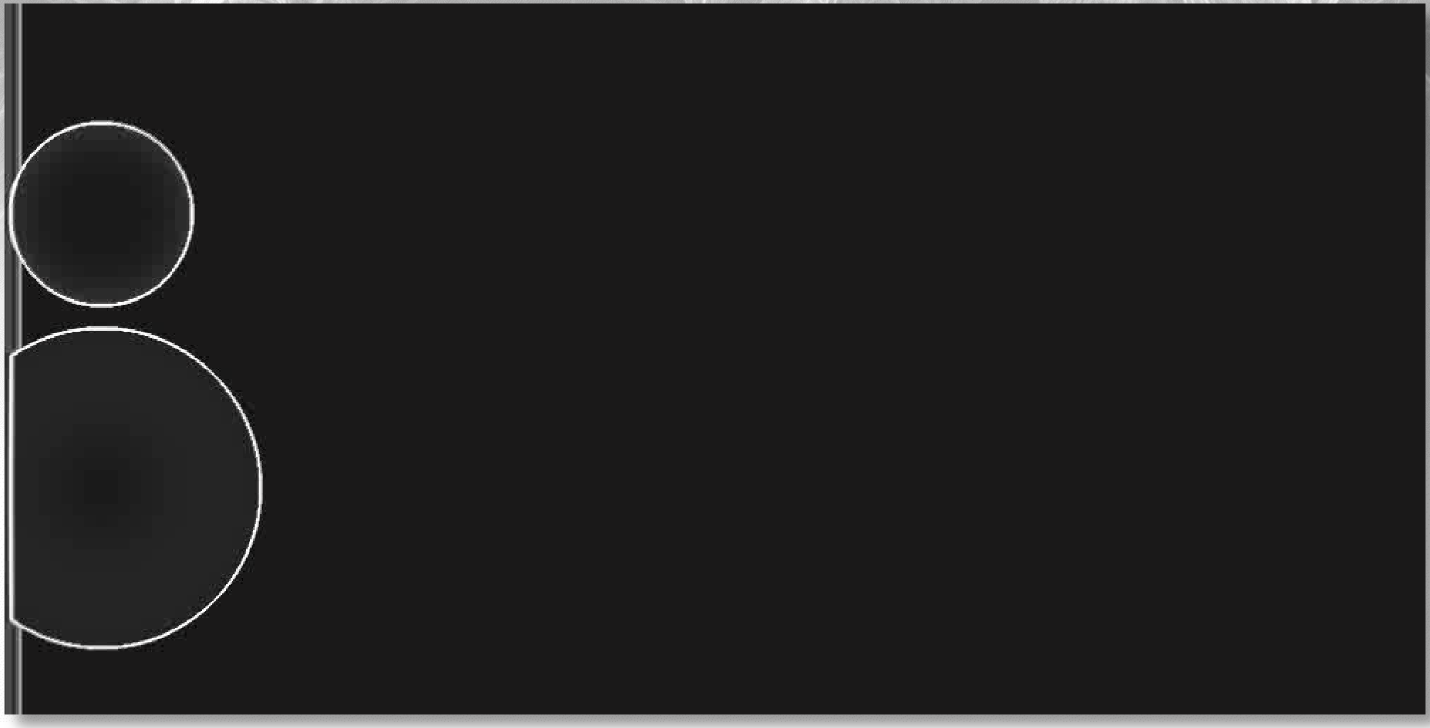




At the last stage of cloud transformation, the conical-like sheets commence to stretch. The flow streams accelerate in high gradient density layers and can initiate whirling of layers at the conventional MCs/ISM borders. Filament rudiments look like the elongated conical folded sheets

k coherent structures evolution in the
d associated with supersonic turbulization.

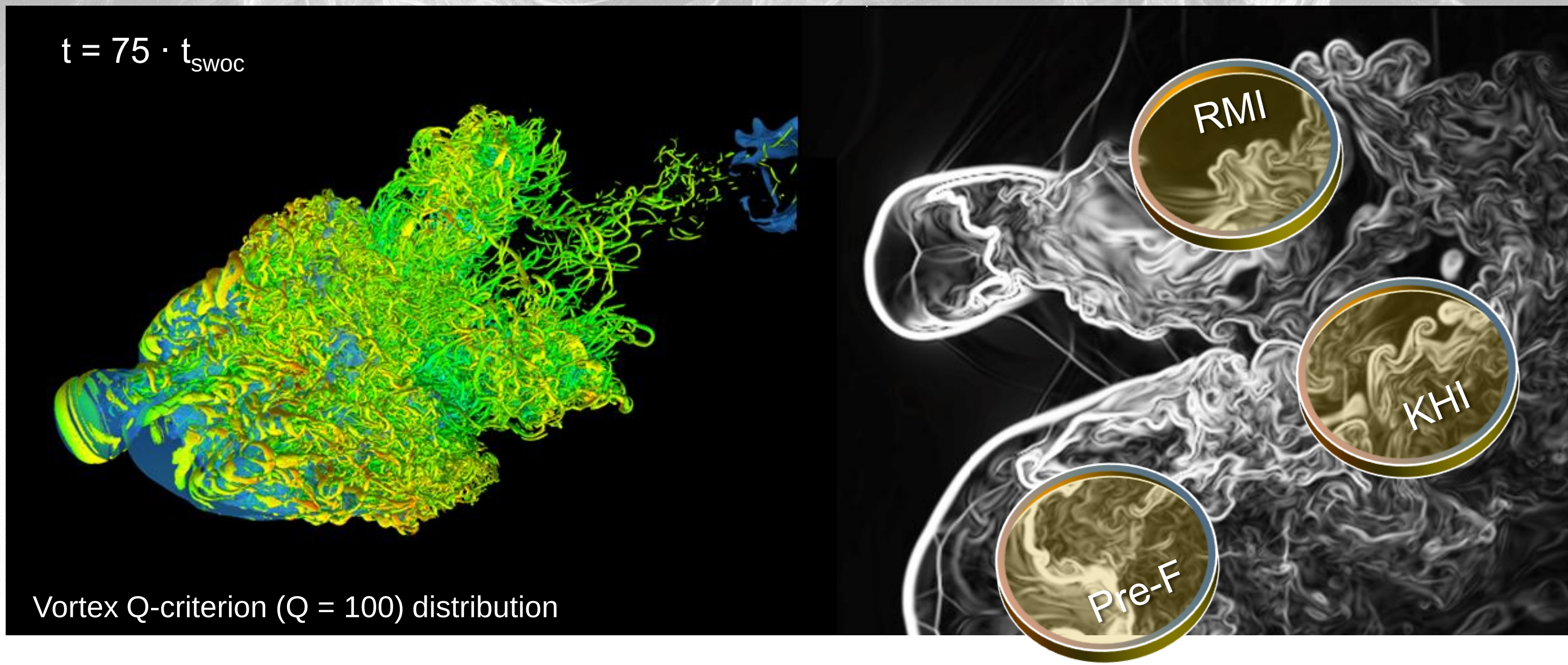
# Numerical schlierens



Schlierens: time sequence from $t = 10 \cdot t_{swoc}$ to $t = 600 \cdot t_{swoc}$

The interference of reflected shock waves and the intensive fluctuations of supersonic velocity fields in gradient zones lead to sharp differentiation of gas density, up to the contrast density ratio $\chi \sim 2000$. Gas compression zones concentrate along film shells of a conventional cylinder-conical form and elongated in the direction of the shock wave propagation.

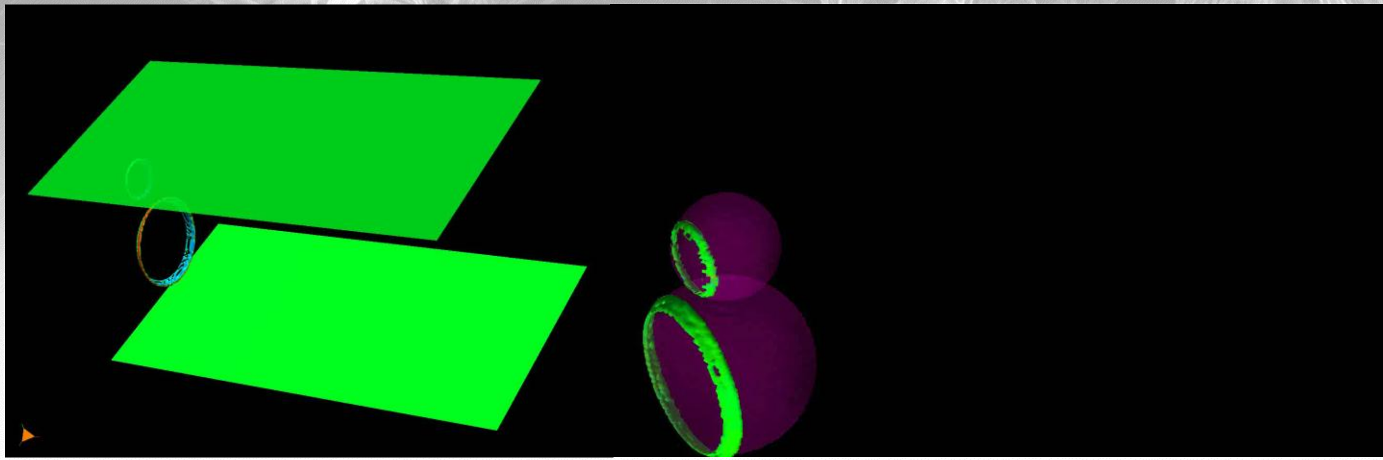
# Richtmyer–Meshkov and Kelvin-Helmholtz instability




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, observed in movie followed.

Vortex sheets start to deflect and twist and become filamented practically after origination of instability.

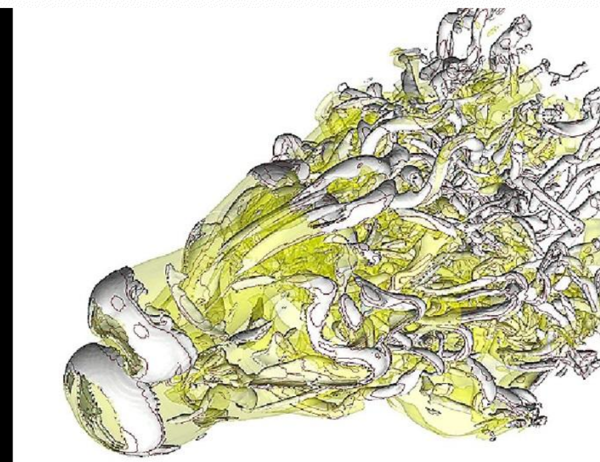
# Vortex structure and time evolution of field of Q – criterion



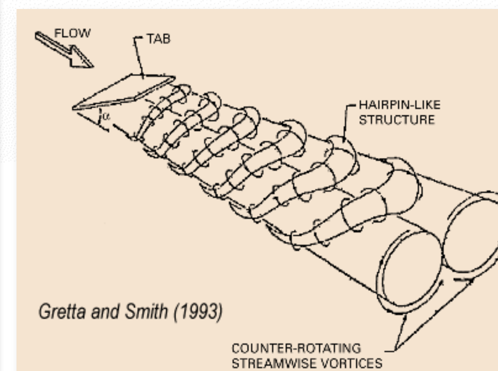
Color indication:
$\omega_x$ – vorticity in the axial direction - mapping on Q-criterion iso-surfaces.

Hunt et al. (1988)

$$\omega_x = \frac{\partial W}{\partial y} - \frac{\partial V}{\partial z}$$



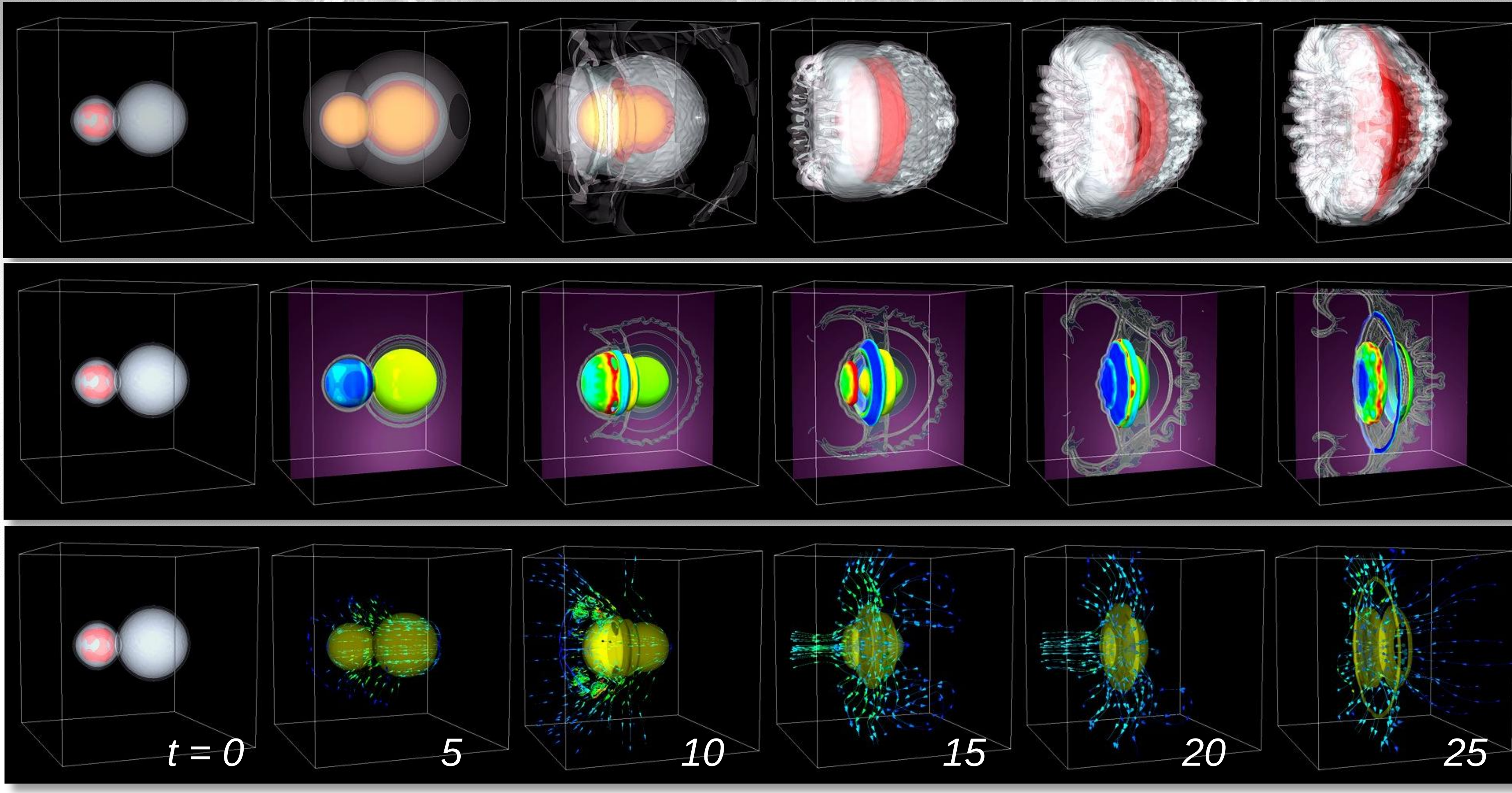
$$Q = \frac{1}{2}\left(u_{i,i}^{\;2} - u_{i,j}u_{j,i}\right) = \frac{1}{2}\left(\|\Omega\|^2 - \|S\|^2\right) > 0$$



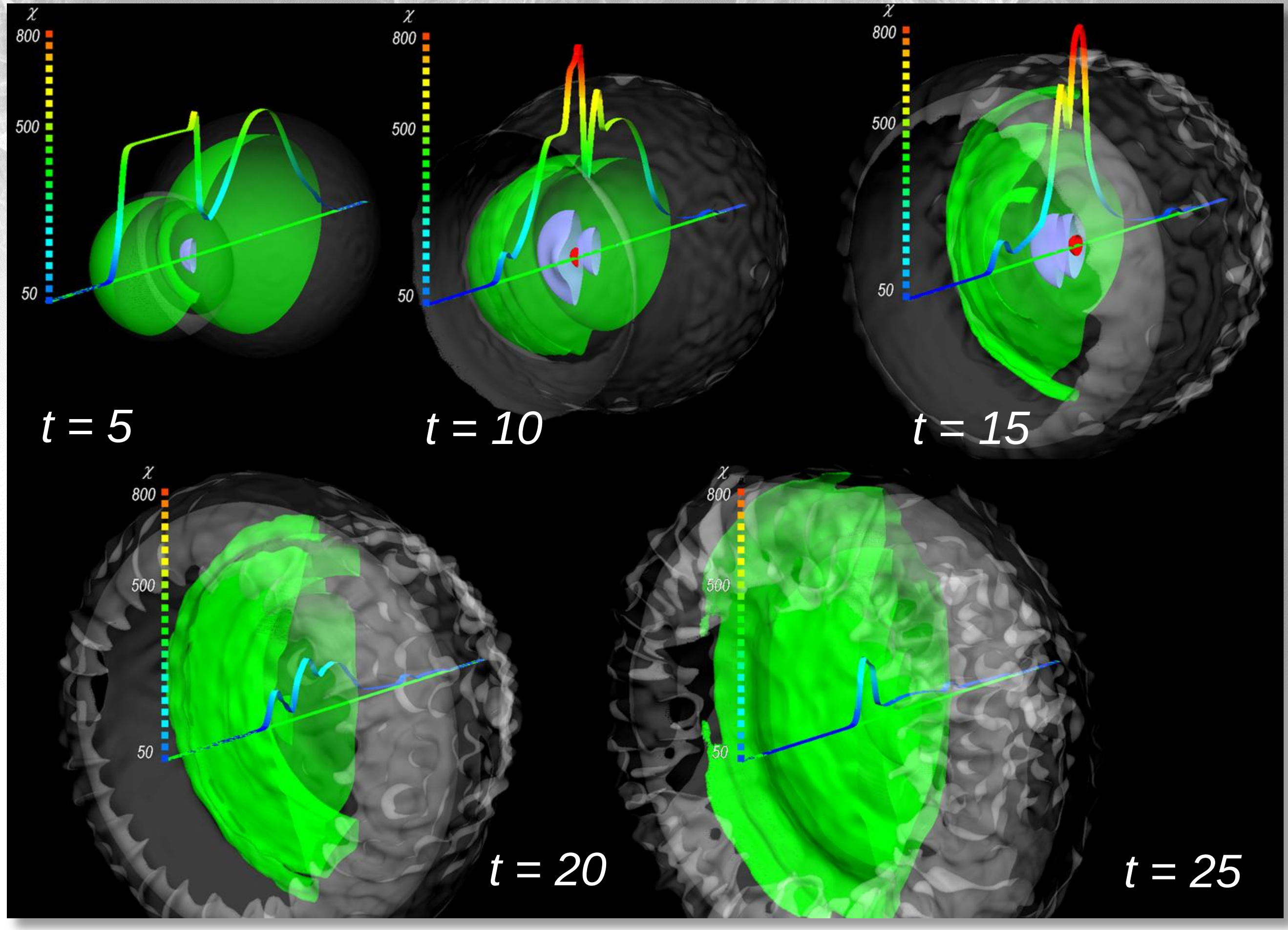

Gretta and Smith (1993)

Figures above show typical vortex formation: with elongated loops and helical deformations inside MCs at the moment of shell forming. One can see that the envelope structures have a recursive fractal distribution. Separate zones are practically eddy-free.

# Case II: temporal evolution of density contrast for MC/MC central impact

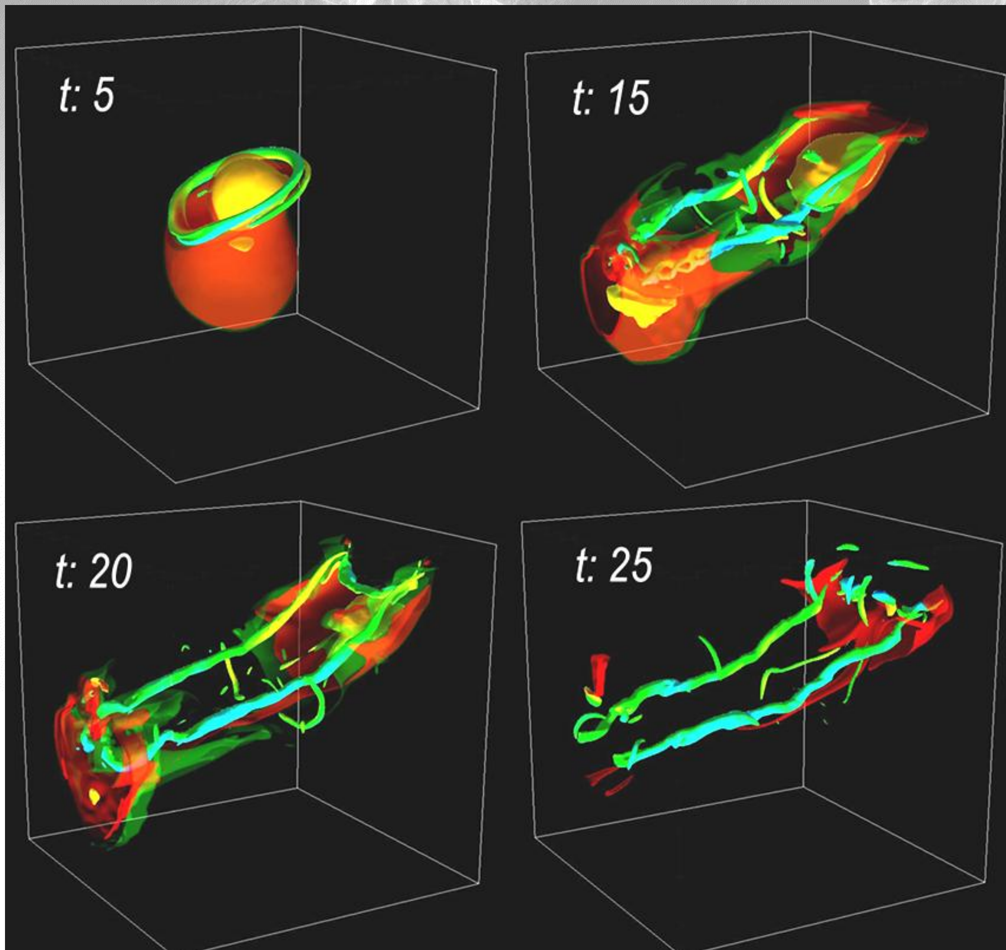


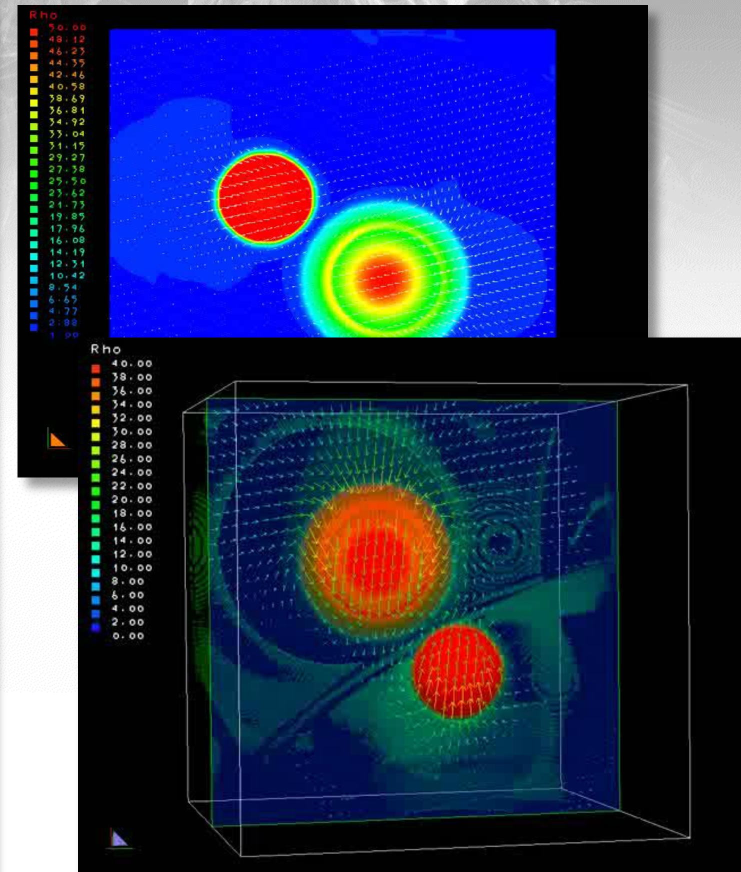
# Case II: Temporal evolution of density contrast for MC/MC central impact




Iso-surfaces $\chi$ = 10, 50, 500, 800 and density contrast profile on the central line.

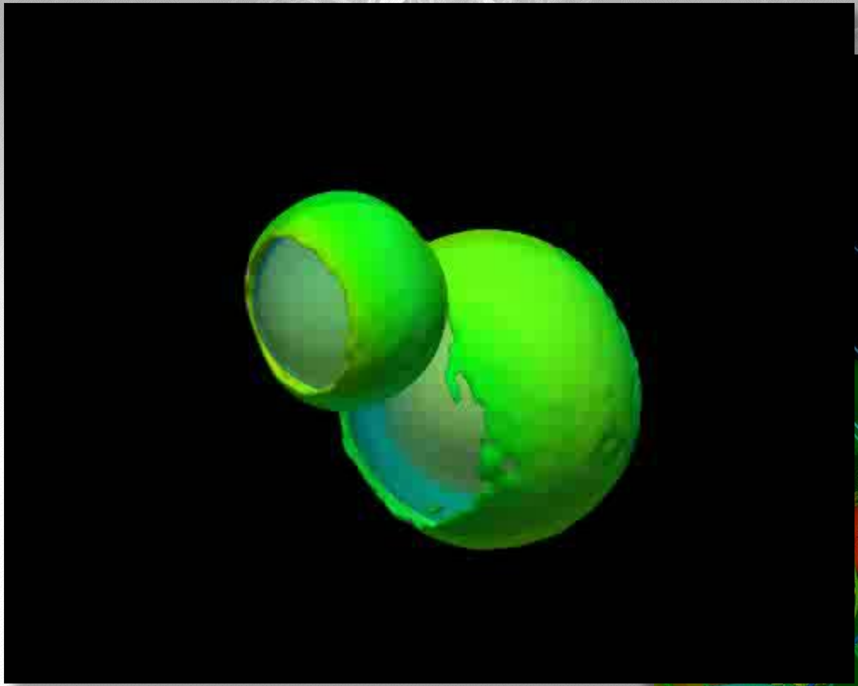
# MC/MC evolution in case III - glancing collision of molecular clouds

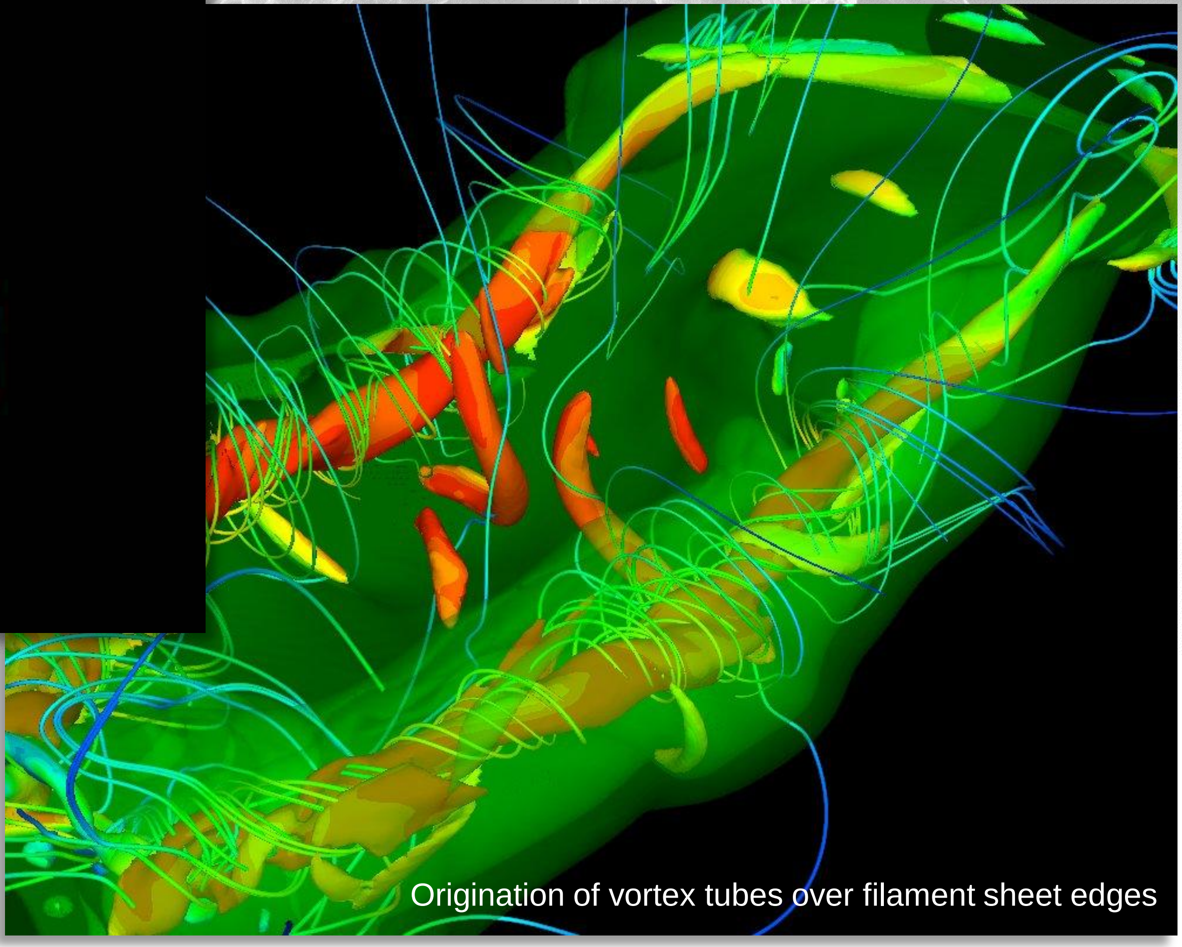



Envelope layers of density contrast $\chi$ = 5, 10, 50 and vortex indicator Q = 5 distribution.

# MC/MC evolution in case III - glancing collision of molecular clouds

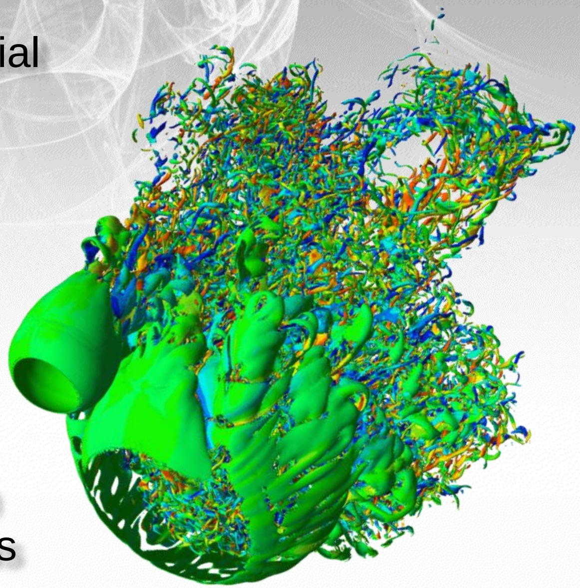




Envelope layers of density contrast
$\chi$ = 5, 10, 30, 50
and indicator Q = 1 and 5 distribution.

Origination of vortex tubes over filament sheet edges

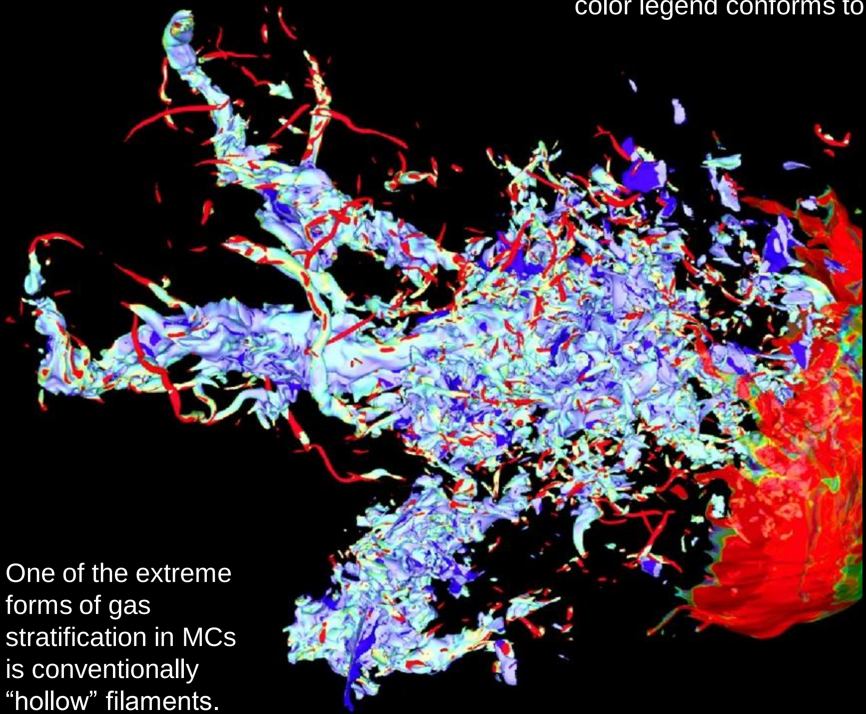
- Filaments forming and molecular clouds crushing were simulated using the HPC numerical modeling with high spatial resolution grids and parallelization codes developed.
- The MCs dynamical transformation for different scenario of molecular clouds collision - between shock wave and MCs and impact between them - were analyzed in terms of supersonic perturbations over shocked sheets as the outcome of local strong shock compression.
- 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
- Assumptions. Filaments are intersection of shocked sheets. Turbulence induces the formation of filaments, which become self-gravitating and can be more fragmented during this process.



Thank you!

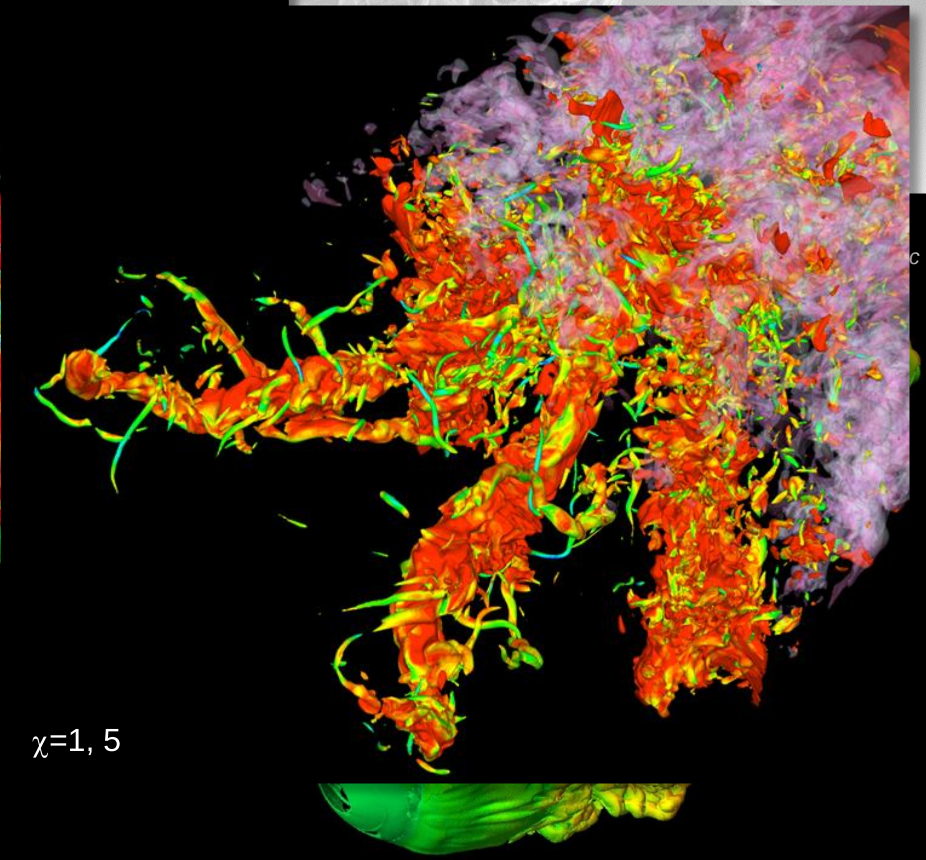
# Vortex structure – denstrophy distribution

Contrast density $\chi$ = 1, 100 with denstrophy contours at t=300$\cdot t_{swoc}$, color legend conforms to 100 < $\Omega_{1/2}$ < 10000.



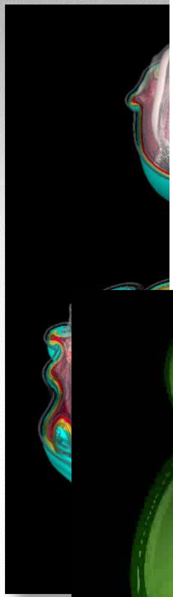
One of the extreme forms of gas stratification in MCs is conventionally “hollow” filaments.

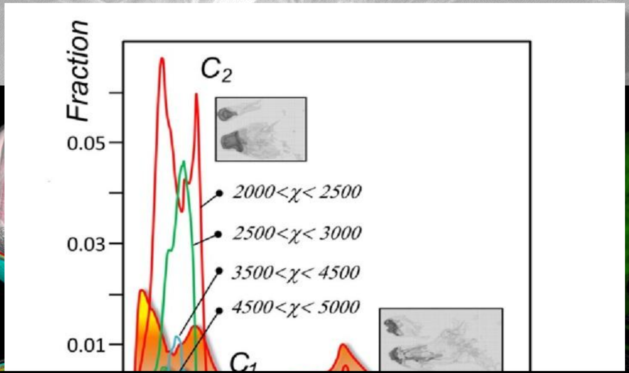
To analyze the vortex nature of MCs transformation and supersonic compression of clouds matter the denstrophy fields were calculated. The local

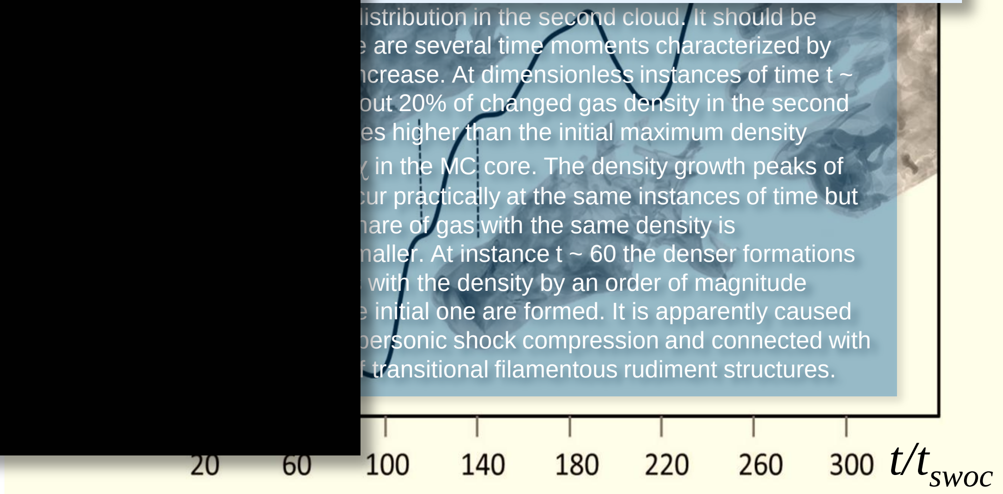


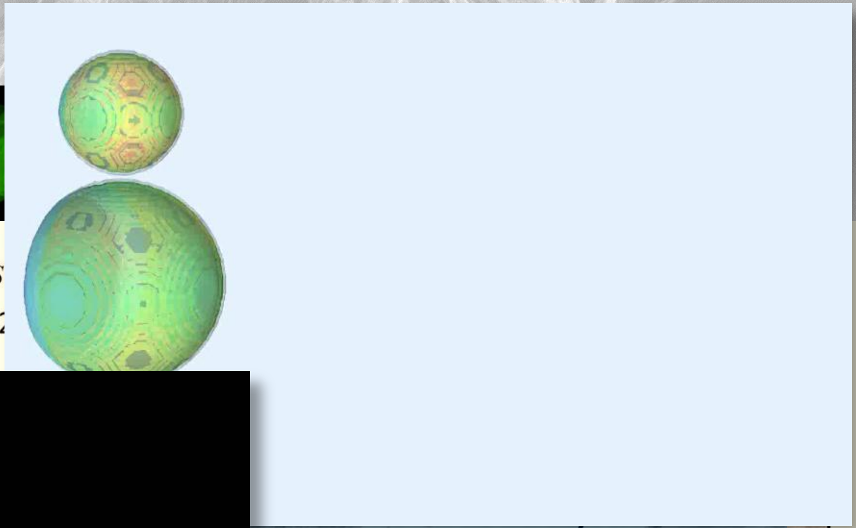

Flow perturbation leads to a considerable grow of the denstrophy over filament envelopes in stripping phase of MCs transformation. Compressed gas sheets assume funneled form. The low-density gas is removed to center zone of cloud formation, and occupy low-pressure regions previously created by rarefaction 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.

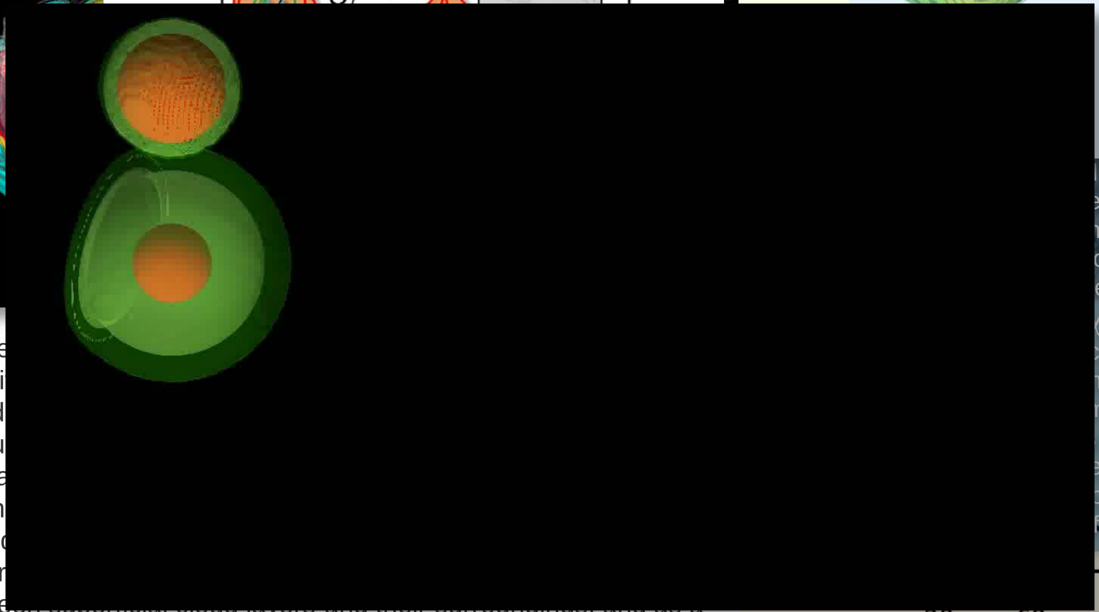
# Drift rate fluctuations during temporal evolution of two clouds







Proce
densi
cloud
fluctu
with a
dimin
period
distur
betwe
consequence drift and crush of clouds can be accelerated.

listribution in the second cloud. It should be
e are several time moments characterized by
ncrease. At dimensionless instances of time t ~
out 20% of changed gas density in the second
es higher than the initial maximum density
χ in the MC core. The density growth peaks of
cur practically at the same instances of time but
hare of gas with the same density is
naller. At instance t ~ 60 the denser formations
with the density by an order of magnitude
e initial one are formed. It is apparently caused
personic shock compression and connected with
f transitional filamentous rudiment structures.