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A new Intel Xeon Phi accelerated hydrodynamic code for numerical simulations of interacting galaxies

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Abstract. In this paper, a new hydrodynamics code to simulate of interacting galaxies on Intel Xeon Phi processors with KNL architecture is presented. A new vector numerical method implemented in the form of a program code for massively parallel architectures is proposed in details. A detailed description is given and a parallel implementation of the code is made. A 92 per cent scalability is reached with 64 processors. The scenarios of interacting galaxies S+E is presented.

1. Introduction

The subject of modern astrophysics is the study of physical processes in the universe, their influence on the self-organization and evolution of astronomical objects, as well as on their further dynamics and interaction. The description of astronomical objects is based on hydrodynamic processes. It is hydrodynamics that determines the nature of astrophysical currents that lead to the evolution of astronomical objects. The impossibility of conducting total experiments leads to the fact that mathematical modeling is the main, and often the only, approach to the theoretical study of astrophysical currents.

The problems of modeling the dynamics of galaxies can be divided by the time of their dynamics. So the evolution of a single galaxy is up to several billion years, while the interaction of individual galaxies is several hundred million years. The movement of galaxies in dense clusters turns collisions between them into an important evolutionary factor, since in the Hubble time a common galaxy can experience up to a dozen collisions with other galaxies of its cluster [1]. Isolated galaxies are important because they have been least affected by interactions over the past billions of years and their morphology is associated with the development of the [2] gravity instability. Thus, the study of both mechanisms of the dynamics of galaxies allows us to explain all their diversity (or in the foreign literature "Galaxy Zoo", with the same project [3]). So, within the framework of this project, the influence of the active galactic nucleus on the formation of galaxies with a bar [4], as well as star formation [5] and stellar mass distribution [6] was studied.

Two reviews of different years are devoted to the main problems of modeling the evolution of galaxies [7, 8]. The main problems that arise in the reviews are questions about the density



profile in galaxies, the rate of star formation, and the rotation speed of galaxies. The problem of the rotation speed profile is raised in connection with the analysis of the Tully-Fisher ratio and the distribution of dark matter in galaxies and the gravitational potential [9]. In the study of the collision of galaxies, it is worthwhile to single out the GALMER project of the Paris Observatory, a database of computational experiments [10] on the collision of various types of galaxies. In processes of collision of galaxies [1] processes (starving [11], Active Galactic Nuclei (AGN) [12], formation of supermassive double black holes [13, 14], chemokinetics [15]) are significantly accelerated and an explicit accounting for these processes in a mathematical model. A similar account must be taken in the problems of evolution of galaxies, for example, a separate collection of papers [16] was devoted to the problem of accounting for various processes in the context of the Galactic Archeology problem of the Milky Way. Most of the subgrid processes occurring in galaxies are described in detail in [17], which will be the basis of this work.

In 2015, we developed the code AstroPhi [18], based on the implementation of the original numerical method using offload programming model Intel Xeon Phi. The accelerator architecture used also did not allow us to implement vector instructions, at the same time the transition to native mode allowed us to get code performance of 28 GigaFlops [19]. Using the low-level vectorization of cycles in the AstroPhi code allowed to obtain the performance increase to the value of the order of 100 GigaFlops [20]. It became clear that it is necessary to use low-level vectorization tools to achieve maximum performance, which was implemented in the new version of the code based on the Harten-Lax-Van Leer (HLL) method and using one [21] accelerator. In this implementation, it was possible to achieve 245 GigaFlops performance on the Intel Xeon Phi 7250 and 302 GFlops on the Intel Xeon Phi 7290. The low order accuracy of the HLL method and the uniprocessor version of the program prompted us to create a new parallel code based on the original numerical method of high accuracy order allowing vectorization calculations. At the same time, we are simultaneously developing code for Intel Xeon Phi with a new numerical method, which is based on a combination of the method of operator separation, Godunov scheme and the modification of the HLL method [22].

The second section of the article is devoted to a description of the mathematical model of interacting galaxies. The third section provides details of the parallel implementation. The fourth section is devoted to the simulation of the collision of galaxies of the types E and S. In the fifth section we formulate the conclusion of the article.

2. Mathematical model

The mathematical model of interacting galaxies is based on the equations of gravitational hydrodynamics for describing the gas component and equations for the first moments of the collisionless Boltzmann equation with the total velocity dispersion tensor for describing the stellar component. The model described in this article is a qualitative extension of the original model from the work [19] taking into account the modern requirements [17], formulated and implemented for the two-dimensional setting.

2.1. Model of gas and stellar components

To describe the gas components, we will use the system of single-speed component gravitational hydrodynamics equations, which is written in Euler coordinates:

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) &= \mathcal{S} - \mathcal{D}, & \frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \vec{u}) &= -s_i + \mathcal{S} \frac{\rho_i}{\rho} - \mathcal{D} \frac{\rho_i}{\rho}, \\ \frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \vec{u}) &= -\nabla p - \rho \nabla (\Phi) + \vec{v} \mathcal{S} - \vec{u} \mathcal{D}, \\ \frac{\partial \rho S}{\partial t} + \nabla \cdot (\rho S \vec{u}) &= (\gamma - 1) \rho^{1-\gamma} (\Lambda - \Gamma) + \rho^\gamma \frac{\mathcal{S}}{\rho} - \rho^\gamma \frac{\mathcal{D}}{\rho}, \end{aligned}$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho E \vec{u}) = -\nabla \cdot (p \vec{v}) - (\rho \nabla(\Phi), \vec{u}) - \Lambda + \Gamma + \rho^\gamma \frac{\mathcal{S}}{\rho} - \rho^\gamma \frac{\mathcal{D}}{\rho},$$

$$\rho E = \frac{1}{2} \rho \vec{u}^2 + \rho \varepsilon, \quad p = (\gamma - 1) \rho \varepsilon = S \rho^\gamma.$$

To describe the collisionless components, we will use the system of equations for the first moments of the Boltzmann collisionless equation, which is also written in Eulerian coordinates:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n \vec{v}) = \mathcal{D} - \mathcal{S}, \quad \frac{\partial n \vec{v}}{\partial t} + \nabla \cdot (n \vec{v} \vec{v}) = -\nabla \Pi - n \nabla(\Phi) + \vec{u} \mathcal{D} - \vec{v} \mathcal{S},$$

$$\frac{\partial n W_{ij}}{\partial t} + \nabla \cdot (n W_{ij} \vec{v}) = -\nabla \cdot (v_i \Pi_j + v_j \Pi_i) - (n \nabla(\Phi), \vec{v}) + \rho^\gamma \frac{\mathcal{D}}{\rho} - \rho^\gamma \frac{\mathcal{S}}{\rho},$$

$$\rho W_{ij} = v_i \times v_j + \Pi_{ij}.$$

The Poisson equation can be written as:

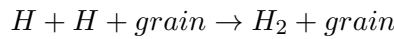
$$\Delta \Phi = 4\pi G(\rho + n),$$

where p – gas pressure, ρ_i – density of i -th species, s_i – speed of formation of i -th species, ρ – density of gas mixture, n – density collisionless component, $\vec{u}$ – speed gas component, $\vec{v}$ – speed collisionless component, ρE – density of total mechanical gas energy, ρW_{ij} – density of total mechanical collisionless components energy, Φ – gravitational potential, ε – density of internal energy of gas, $\mathcal{S}$ – entropy, γ – adiabatic index, Π_{ij} – a tensor of dispersion of speeds collisionless components, $\mathcal{S}$ – the speed of formation of supernova stars, $\mathcal{D}$ – star formation speed, Λ – function of Compton cooling, Γ – function of heating from explosion of supernova stars. The subgrid processes will be describe in next subsections.

2.2. Chemical reactions

The following eight reactions, that was also used in work [27], was examined.

- (i) Molecular hydrogen formation [28]:



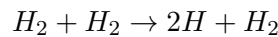
which held with speed k_1 and initiate heating of Γ_1 .

- (ii) Molecular hydrogen first dissociation [29]:



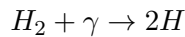
which held with speed k_2 and initiate heating of Λ_2 .

- (iii) Molecular hydrogen second dissociation [30]:



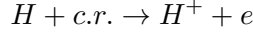
which held with speed k_3 and initiate cooling of Λ_3 .

- (iv) Molecular hydrogen photodissociation [27]:



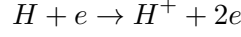
which held with speed k_4 and initiate heating of Γ_4 .

(v) Cosmic Ray ionization [27]:



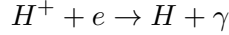
which held with speed k_5 and initiate heating of Γ_5 .

(vi) Collision ionization [31]:



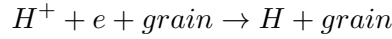
which held with speed k_6 and initiate cooling of Λ_6 .

(vii) Radiative recombination [32]:



which held with speed k_7 and initiate cooling of Λ_7 .

(viii) EI recombination on grains [33]:



which held with speed k_8 and initiate cooling of Λ_8 .

Effective adiabatic index was used in the following form:

$$\gamma = \frac{5n_H + 5n_e + 7n_{H_2}}{3n_H + 3n_e + 5n_{H_2}}$$

2.3. The processes of star formation and the effect of supernova explosions

The supernovae feedback we should use for SNII, SNIa and other stars by stellar wind $\mathcal{S} = \mathcal{S}_{SNII} + \mathcal{S}_{SNIa} + \mathcal{S}_*$. For describe of supernova feedback we should use the initial mass function [24]

$$\phi(M_*) = \begin{cases} AM_*^{-1.3}, & M_* \leq 0.5M_\odot \\ AM_*^{-2.3}, & M_* > 0.5M_\odot \end{cases}$$

stellar lifetimes function [25]

$$\tau(M_*) = \begin{cases} 1.2M_*^{-1.85} + 0.003Gyr, & M_* \geq 7.45M_\odot \\ 10^{f(M_*)}, & M_* < 7.45M_\odot \end{cases}$$

where

$$f(M_*) = \frac{0.334 - \sqrt{1.79 - 0.2232 \times (7.764 - \log(M_*))}}{0.1116}$$

and nucleosynthes [26]. For each type of stars their share is determined $\mathcal{R}_{II, Ia, *}$ (see details in work [17]) and the rate of star formation is determined by the simple formula:

$$\mathcal{S} = \rho \times (\mathcal{R}_{SNII} + \mathcal{R}_{SNIa} + \mathcal{R}_*)$$

We note that the supernova explosion also contributes to the heating of the gas

$$\Gamma = 10^{51} \times (\mathcal{R}_{SNII} + \mathcal{R}_{SNIa}) \times M_\odot \times V^{-1}$$

The rate of star formation is taken from work [19].

2.4. Cooling and heating functions

The contribution to the cooling and heating functions is made by chemistry, which was described in the previous subsection, as well as supernovae feedback, in the following we will consider other sources of cooling/heating.

We will consider cooling functions in two temperature modes:

- (i) The low-temperature cooling. At low temperatures, the ionization of the elements H, O, C, N, Si, and Fe occurs due to collision. The collision frequency and the corresponding cooling function can be found in the work [34].
- (ii) The high-temperature cooling. At high temperatures, the emission process for the elements H, He, C, N, O, Ne, Mg, Si, and Fe occurs. The cooling function can be found in paper [35].

To describe the heating function, we will consider the following two processes:

- (i) Cosmic ray heating. The process of ionization of hydrogen and helium atoms. The heating function can be found in operation [36].
- (ii) Photoelectric heating from small dust grains [37].

3. Parallel numerical solution method

To solve the hydrodynamic equations, we use a combination of the HLL method with a piecewise parabolic representation of the solution [23]. To solve the Poisson equation, a fast Fourier transform method is used.

3.1. Numerical method for solving equations of hydrodynamics of high order of accuracy

Equations for describing the gas and stellar components without taking into account the right-hand side can be written in a single vector form:

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0$$

To solve the equations, we used the HLL method, modified taking into account the piecewise parabolic representation of the solution. The flow across the boundary between the left (L) and right (R) cells is calculated by the equation:

$$F_{HLL} = \frac{\lambda_R F(-\lambda_L \tau) - \lambda_L F(\lambda_R \tau) + \lambda_R \lambda_L (U(-\lambda_L \tau) - U(\lambda_R \tau))}{\lambda_R - \lambda_L}$$

where

$$\lambda_L = \min \left(0; u_L - \sqrt{\gamma S_L \rho_L^{\gamma-1}} \right) \quad \lambda_R = \max \left(0; u_R + \sqrt{\gamma S_R \rho_R^{\gamma-1}} \right)$$

The integration over parabolas is carried out by the equations described in the work [23]. We will describe in detail the implementation of the equations for constructing parabolas and the formation of a flow vector further in describing the vectorization of computations.

3.2. The method of solving the Poisson equation

After solving the hydrodynamic equations, it is necessary to restore the gravitational potential according to the densities of the gas and collisionless components. To do this, we will use a 27-point template to approximate the Poisson equation. This is due to the fact that the solution with respect to rotation is maximally invariant. The algorithm for solving the Poisson equation will consist of several stages:

- (i) Setting the boundary conditions for the gravitational potential at the boundary of the region based on the use of the first terms of the multipole expansion - static, axial and centrifugal moments of inertia.
- (ii) The transformation of density into harmonic space. The resulting density is represented as a superposition of eigenfunctions of the Laplace operator:

$$\rho_{i,k,l} + n_{i,k,l} = \sum_{jmn} \sigma_{jmn} \exp \left(\frac{\vec{i}\pi j}{I} + \frac{\vec{i}\pi km}{K} + \frac{\vec{i}\pi ln}{L} \right)$$

where I, K, L – the number of cells in each coordinate, $\vec{i}$ – imaginary unit. For this, a fast Fourier transform is used.

- (iii) Solution of the Poisson equation in harmonic space using a fairly simple formula for calculating the amplitudes of the potential harmonics:

$$\phi_{jmn} = \frac{\frac{2}{3}\pi h^2 \sigma_{jmn}}{1 - \left(1 - \frac{2\sin^2 \frac{\pi j}{I}}{3}\right) \left(1 - \frac{2\sin^2 \frac{\pi m}{K}}{3}\right) \left(1 - \frac{2\sin^2 \frac{\pi n}{L}}{3}\right)}$$

After that it is necessary to perform the inverse fast Fourier transformation of the potential harmonics into the functional space of the harmonics.

3.3. Accounting for subgrid processes

Subgrid processes are accounted for using the Euler method for solving ordinary differential equations (ODE).

3.4. Regularization of the solution

At the final stage of the hydrodynamic equations, a solution adjustment procedure is provided. In the case of a gas vacuum border:

$$|\vec{u}| = \sqrt{2(E - \epsilon)}, (E - \vec{u}^2/2)/E \geq 10^{-3},$$

In the other area, an adjustment is used to guarantee non-decreasing entropy:

$$|\rho\epsilon| = \left(\rho E - \frac{\rho \vec{u}^2}{2} \right), (E - \vec{u}^2/2)/E < 10^{-3},$$

This modification provides a detailed balance of energy and guarantees non-decreasing entropy.

3.5. Geometric decomposition of the computational domain

Using a uniform grid in Cartesian coordinates to solve the equations of hydrodynamics makes it possible to use an arbitrary Cartesian topology for decomposition of the computational domain. Such organization of calculations has potentially infinite scalability. The code uses a multilevel one-dimensional decomposition of the computational domain. At one coordinate, the external one-dimensional cutting takes place using the MPI technology, within each subdomain, cutting takes place using OpenMP tools adapted for Intel Many Integrated Core (MIC) architectures, vectorization of calculations using AVX-512 is used on each core. A similar approach was also used in the first version of the program code AstroPhi [18] taking into account the use of offload mode.

3.6. Research code performance

A code scalability study was performed on the mesh $256p \times 256 \times 256$ using all logical cores for each accelerator, where p – is the number of accelerators used. Thus, for each accelerator, the size of the subdomain is 256^3 . To study the scalability, the time of the numerical method in seconds (Total) was measured with different number of used Intel Xeon Phi (MIC) accelerators. The scalability of T (Scalability) was calculated using the formula

$$T = \frac{Total_1}{Total_p}$$

where $Total_1$ – is the computation time for one accelerator using one accelerator, $Total_p$ – is the computation time for one accelerator using p accelerators. The results of acceleration studies are shown in figure 1. Thus, using all 64 accelerators 92 % efficiency was obtained, which is a

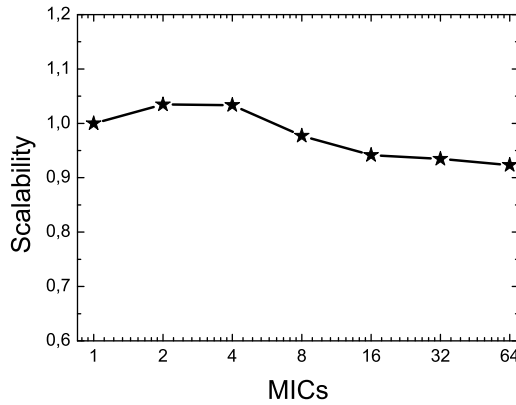


Figure 1. Code Scalability for Different Number of Intel Xeon Phi Accelerators

fairly high result.

3.7. Vectorization of a numerical method using AVX 512

For the vectorization of calculations, AVX-512 technology is used, the scheme for vectorizing formulas for constructing and using parabolas and the functions used for this are shown in the figure 2. The flow computation is vectorized trivially and is described in work [21].

4. Simulation of the collision of galaxies S and E types

We will simulate the collision of two galaxies with a mass $M = 10^{13} M_{\odot}$ and velocity $v_{cr} = 800$ km/s, the first of which is given by self-gravitating spherical clouds to describe the gas and collisionless components with an equilibrium initial density distribution, pressure / tensor of velocity dispersion. The stellar component of the second galaxy has a spiral shape. Galaxies rotate in opposite directions with differential rotation:

$$v_{\phi} = \sqrt{r \frac{\partial \Phi}{\partial r}}$$

The figure 3 presents the results of the distribution of the column density of the gas and stellar components. After the collision process behind the front of the shock wave, the star formation rate increases actively, and molecular hydrogen is formed at the site of the future galaxy. It

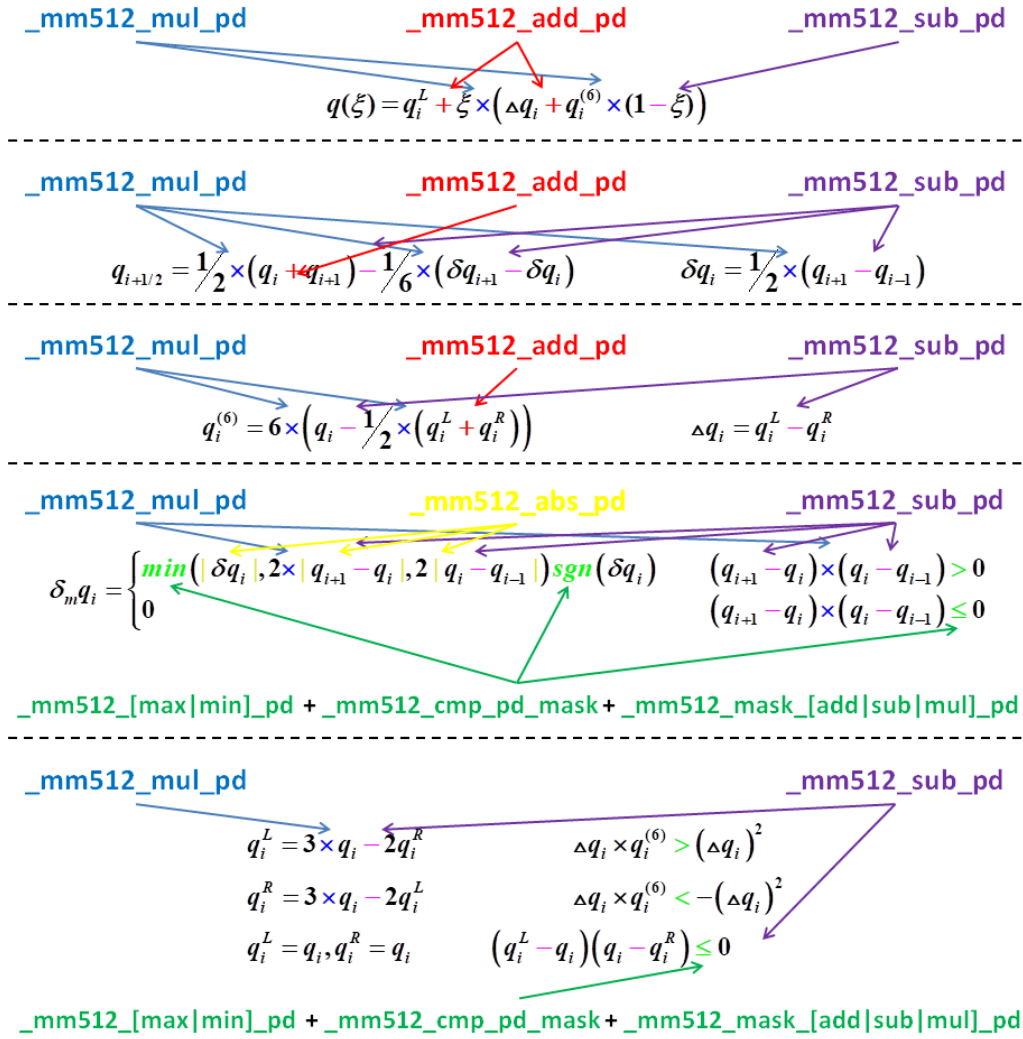


Figure 2. Scheme of vectorization of calculations

should be noted that the growth of formation is observed in the region corresponding to the spiral form. Probably, with explicit account of the process of star formation in the model, it is possible to simulate the formation of a spiral galaxy as a result of a collision of a spiral galaxy and a disk galaxy.

5. Conclusion

The paper presents a new hydrodynamic code for simulating the collision of galaxies on supercomputers equipped with Intel Xeon Phi accelerators. The mathematical model of interacting galaxies is based on the equations of gravitational hydrodynamics for describing the gas component and equations for the first moments of the collisionless Boltzmann equation with the total velocity dispersion tensor for describing the stellar component. The construction and investigation of a parallel computational method for solving the equations of hydrodynamics are described in detail. A 92 percent scalability is reached with 64 processors. The scenarios of interacting galaxies S+E is presented.

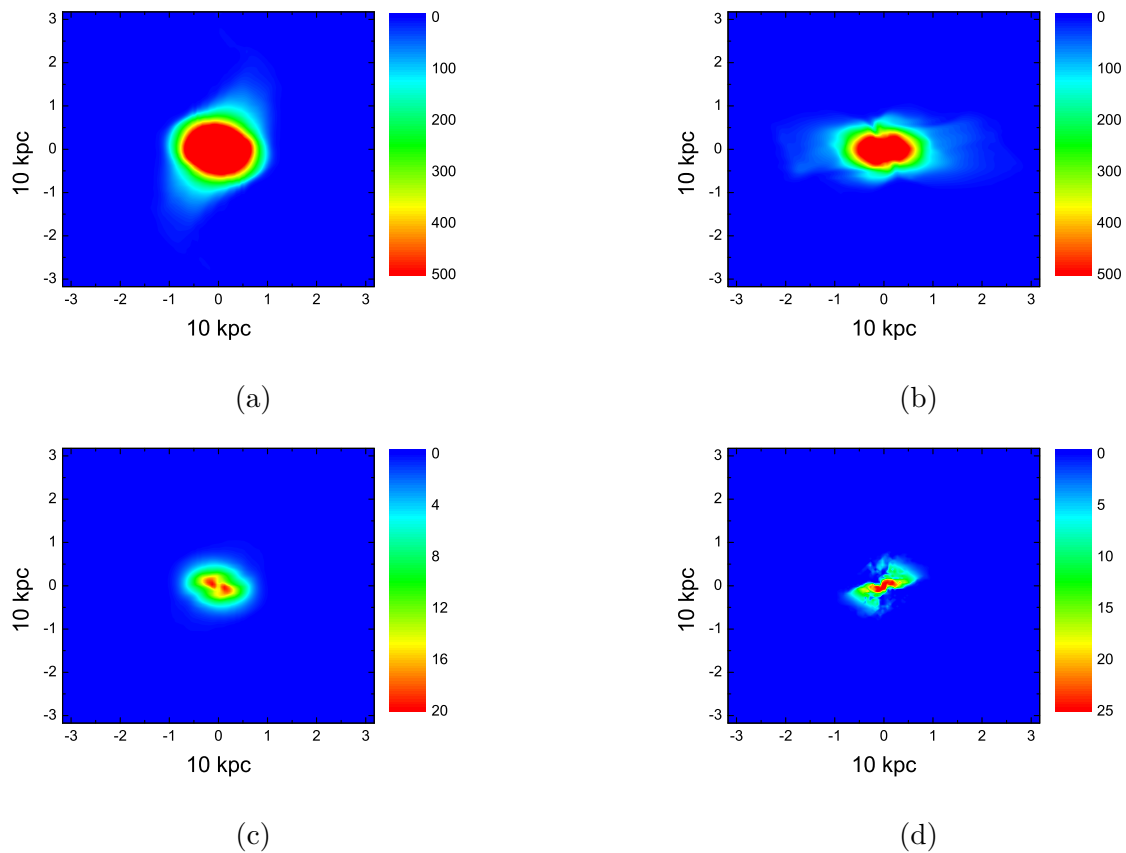


Figure 3. The column density in $M_{\odot}pc^{-2}$ at the time $t = 400$ Myr of the gas component (a), the stellar component (b), molecular hydrogen (c). The rate of the star formation process $M_{\odot}pc^{-2}Myr^{-1}$ at time $t = 400$ Myr – (d).

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