Simulation of formaldehyde formation during a galaxy collision using vectorized numerical method on Intel Xeon Phi accelerators

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Abstract. Implementation of a new vectorized high-order accuracy numerical method for solving gravitational gas dynamics equations on supercomputers equipped with Intel Xeon Phi accelerators is presented in the paper. Combination of the Godunov method, the Harten-Lax-Van Leer method and the piecewise parabolic method on local stencil is at the basis of the method, that allows achieving high-order accuracy for smooth solutions and low dissipation on discontinuities. Chemokinetic model of formaldehyde formation based on molecular hydrogen and carbon monoxide is presented. Numerical experiment results, which describe the mechanism of formaldehyde formation based on reactions involving molecular hydrogen and carbon monoxide during a collision of different types of galaxies, are shown.

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 character of astrophysical flows, which leads to the evolution of astrophysical objects. Mathematical modeling is the main and often the only way for theoretical investigation of astrophysical flows due to the impossibility of carrying out total experiments.

Problems of modeling of galaxies dynamics could be divided by its duration. 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 gravity instability [2]. Thus, the study of both mechanisms of the dynamics of galaxies allows us to explain all their diversity.

In the galaxies collision problems [1], all processes (star formation [3], AGN [4], supermassive black holes formation [5, 6], chemokinetics [7]) are significantly accelerated and explicit accounting of them in a mathematical model is necessary. The major part of the subgrid processes occurring in galaxies are described in details in [8], which in the basis of the project.

2. Mathematical model

Mathematical model of interacting galaxies is based on gravitational gasdynammics equations to describe the gas component, and equations for the first momenta of the collisionless Boltzmann equation with full tensor of velocities dispersion to describe the star component. The model described in the paper is a qualitative extension of the original model from [9] which taking into account the modern requirements [8] defined and implemented in two-dimensional formulation.

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

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = \mathcal{S} - \mathcal{D}, \qquad \frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \vec{u}) = -s_i + \mathcal{S}\frac{\rho_i}{\rho} - \mathcal{D}\frac{\rho_i}{\rho},$$

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

$$\frac{\partial \rho S}{\partial t} + \nabla \cdot (\rho S \vec{u}) = (\gamma - 1)\,\rho^{1-\gamma}\,(\Lambda - \Gamma) + \rho^{\gamma}\frac{\mathcal{S}}{\rho} - \rho^{\gamma}\frac{\mathcal{D}}{\rho},$$

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

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

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:

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

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

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

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, 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 described further.

The following four reactions, that were also used in work [10], were examined.

(i) Molecular hydrogen formation [11]:

$$H + H + grain \rightarrow H_2 + grain$$

(ii) Molecular hydrogen first dissociation [12]:

$$H_2 + H \rightarrow 3H$$

(iii) Molecular hydrogen second dissociation [13]:

$$H_2 + H_2 \to 2H + H_2$$

(iv) Formaldehyde formation [14]:

$$H_2 + CO \to H_2CO$$

Cooling functions will be considered in the low-temperature cooling regime [15] and the high-temperature cooling regime [16]. To describe heating functions the cosmic ray heating [17] and photoelectric heating from small dust grains [18] will be used.

3. Parallel numerical method

The combination of HLL with piecewise-parabolic representation of the solution [19] is used for solving the hydrodynamics equations. The method based on Fast Fourier Transform is used for solving the Poisson equation. Subgrid processes are considered with help of Euler method for solving of an ODE. At the final stage of the hydrodynamic equations, a solution adjustment procedure is provided. This modification provides a detailed balance of energy and guarantees non-decreasing entropy.

Multilevel one-dimensional decomposition of the computational domain is used in the code. External one-dimensional cutting by one of the coordinates is done with MPI technology, and inside of each subdomain cutting is done with OpenMP adapted for MIC architectures. On each core vectorization of calculations with AVX-512 is used [20].

4. Simulation of S and E types of galaxies collision

Let us simulate the collision of two galaxies with mass $M = 10^{13} M_{\odot}$ and velocity $v_{cr} = 800$ kmps. The first one is described by self-gravitating spherical clouds for gas and collisionless components with an equilibrium initial distribution of density, pressure/velocity dispersion tensor. The stellar component of the second one has spiral form.

There is a molecular hydrogen formation in areas with high density in the center of a new galaxy after the main phase of the galaxies collision. We used the CO concentration typical for observations in such areas, and formation of the formaldehyde was modeled according to obtained concentrations. In the presentation we will show the mechanism of H_2CO formation in interacting galaxies in details.

5. Conclusion

The new hydrodynamical code for modeling of the galaxies collision on supercomputers equipped with Intel Xeon Phi is presented in the paper. 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 structure of the parallel numerical method for solving the hydrodynamics equations is described. The scenarios of interacting galaxies S+E is presented.

6. References

[1] Tutukov, A. Gas Dynamics of a Central Collision of Two Galaxies: Merger, Disruption, Passage, and the Formation of a New Galaxy / A. Tutukov, G. Lazareva, I. Kulikov // Astronomy Reports. – 2011. – Vol. 55(9). – P. 770-783.

[2] Khim, H. Demographics of Isolated Galaxies along the Hubble Sequence // The Astrophysical Journal Supplement Series. – 2015. – Vol. 220(1). – P. 3.

[3] Schweizer, F. Merger-Induced Starbursts // Astrophysics and Space Science Library. – 2005. – Vol. 329. – P. 143-152.

[4] Sol Alonso, M. Active galactic nuclei and galaxy interactions / M. Sol Alonso, D. Lambas, P. Tissera, G. Coldwell // Monthly Notices of the Royal Astronomical Society. – 2007. – Vol. 375(3). – P. 1017-1024.
[5] Blecha, L. Double-peaked narrow-line signatures of dual supermassive black holes in galaxy merger simulations / L. Blecha, A. Loeb, R. Narayan // Monthly Notices of the Royal Astronomical Society. – 2013. – Vol. 429(3). – P. 2594-2616.
[6] Rodriguez, C. Hi observations of the supermassive binary black hole system in 0402+379 / C. Rodriguez, G. Taylor, R. Zavala, Y. Pihlstrom, A. Peck // The Astrophysical Journal. – 2009. – Vol. 697(1). – P. 37-44.
[7] Combes, F. Chemodynamical evolution of interacting galaxies / F. Combes, A. Melchior // Astrophysics and Space Science. – 2002. – Vol. 281(1-2). – P. 383-387.
[8] Vorobyov, E. Stellar hydrodynamical modeling of dwarf galaxies: simulation methodology, tests, and first results / E. Vorobyov, S. Recchi, G. Hensler // Astronomy & Astrophysics. – 2015. – Vol. 579. – P. A9.
[9] Kulikov, I. A New Hydrodynamic Model for Numerical Simulation of Interacting Galaxies on Intel Xeon Phi Supercomputers / I. Kulikov, I. Chernykh, A. Tutukov // Journal of Physics: Conference Series. – 2016. – Vol. 719. – P. 012006.
[10] Glover, S. Simulating the Formation of Molecular Clouds. I. Slow Formation by Gravitational Collapse from Static Initial Conditions / S. Glover, M. Mac Low // The Astrophysical Journal Supplement Series. – 2007. – Vol. 169(2). – P. 239-268.
[11] Hollenbach, D. Molecule formation and infrared emission in fast interstellar shocks. I Physical processes / D. Hollenbach, C.F. McKee // The Astrophysical Journal Supplement Series. – 1979. – Vol. 41. – P. 555-592.
[12] Lepp, S. The kinetic theory of H2 dissociation / S. Lepp, J.M. Shull // The Astrophysical Journal. – 1983. – Vol. 270. – P. 578-582.
[13] Martin, P. Collision-induced Dissociation of Molecular Hydrogen at Low Densities / P. Martin, W. Keogh, M. Mandy // The Astrophysical Journal. – 1998. – Vol. 499. – P. 793-798.
[14] Vichietti, R. The H2 + CO ↔ H2CO Reaction: Rate Constants and Relevance to Hot and Dense Astrophysical Media / R. Vichietti, R. Spada, A. Da Silva, F. Machado, R. Haiduke // The Astrophysical Journal Supplement Series. – 2016. – Vol. 225 – P. 7.
[15] Dalgarno, A. Heating and Ionization of HI Regions / A. Dalgarno, R.A. McCray // Annual Review of Astronomy and Astrophysics. – 1972. – Vol. 10. – P. 375-426.
[16] Boehringer, H. Metallicity-dependence of radiative cooling in optically thin, hot plasmas / H. Boehringer, G. Hensler // Astronomy & Astrophysics. – 1989. – Vol. 215(1). – P. 147-149.
[17] Van Dishoeck, E.F. Comprehensive models of diffuse interstellar clouds - Physical conditions and molecular abundances / E.F. Van Dishoeck, J.H. Black // The Astrophysical Journal Supplement Series. – 1986. – Vol. 62. – P. 109-145.
[18] Bakes, E.L.O. The photoelectric heating mechanism for very small graphitic grains and polycyclic aromatic hydrocarbons / E.L.O. Bakes, A.G.G.M. Tielens // The Astrophysical Journal. – 1994. – Vol. 427(2). – P. 822-838.
[19] Kulikov, I. Using the PPML approach for constructing a low-dissipation, operator-splitting scheme for numerical simulations of hydrodynamic flows / I. Kulikov, E. Vorobyov // Journal of Computational Physics. – 2016. – Vol. 317. – P. 318-346.
[20] Kulikov, I.M. An Efficient Optimization of HLL Method for the Second Generation of Intel Xeon Phi Processor / I.M. Kulikov, I.G. Chernykh, B.M. Glinskiy, V.A. Protasov // Lobachevskii Journal of Mathematics. – 2018. – Vol. 39(4). – P. 543-550.

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