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

I Kulikov\textsuperscript{1}, I Chernykh\textsuperscript{1}, V Protasov\textsuperscript{1} and I Gubaydullin\textsuperscript{2}

\textsuperscript{1}Institute of Computational Mathematics and Mathematical Geophysics SB RAS, Lavrentyev av. 6, Novosibirsk, Russia, 630090
\textsuperscript{2}Institute of Petrochemistry and Catalysis RAS, Oktyabrya av. 141, Ufa, Russia, 450075

e-mail: chernykh@parbz.sscc.ru

\textbf{Abstract.} We present implementation of a new vectorized high-order accuracy numerical method for solving gravitational hydrodynamics equations on supercomputers equipped with Intel Xeon Phi in the paper. Combination of the Godunov method, the Harten-Lax-Van Leer method and the piecewise parabolic method on the local stencil is at the basis of the method. It allows achieving high-order accuracy for smooth solutions and low dissipation on discontinuities. We present chemokinetic model of formaldehyde formation based on molecular hydrogen and carbon monoxide. We show the results of numerical simulation of interacting galaxies.

1. Introduction
It is possible to divide problems of modeling of galaxies dynamics 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. For the Hubble time a common galaxy can experience up to a dozen collisions with other galaxies of its cluster [1]. Isolated galaxies are also important because they are least affected by interactions over the past billions of years and their morphology is associated with the development of the gravitational 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], chemokinetic [7]) are significantly accelerated. Therefore, it is necessary to explicitly account them in a mathematical model. The work [8] describes the major part of the subgrid processes occurring in galaxies in details which are in the basis of the project.

The galaxies collisions in the model of the N-body gravitational interaction has a limitation on the ability to reproduce different types of galaxies. This is especially relevant for peculiar galaxies which formation mechanism is based on the interaction of galaxies. Observations show that the gas component plays a significant role in the galaxies collision. Gas component parameters with the same stellar component may lead to different scenarios of collisions: dispersion, merger, free pass, pass with formation of a third new galaxy. Certainly, consideration of the gas component requires significantly increase computational resources. Incorporation of
the subgrid processes and chemical reaction is quite important. The need for effective use of computational resources pushed us to utilize all the available computational technologies for solving astrophysical problems. While using the Intel Xeon Phi accelerators the main source of computations performance increase is vectorization. In this connection, we developed the code with the usage of low-level vectorization tools. This capability has no analogues in the World for solving problems of astrophysics.

2. The Physics Model

In the basis of the numerical model of interacting galaxies are gravitational gasdynamics equations to describe the gas component, and equations for the first moments of the collisionless Boltzmann equation with the full tensor of velocities dispersion to describe the star component. The model we describe in the paper is a qualitative extension of the original model from [9]. It takes into account the modern requirements [8] defined and implemented in the two-dimensional formulation.

2.1. Hydrodynamical Model of Galaxies

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

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = S - D, \quad \frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \vec{u}) = -s_i + \rho \frac{\rho_i}{\rho} - D \frac{\rho_i}{\rho},
\]

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

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

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

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

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

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

\[
\frac{\partial n \Pi_{ij}}{\partial t} + \nabla \cdot (n \Pi_{ij} \vec{v}) = -\nabla \cdot (v_i \Pi_j + v_j \Pi_i) - (n \nabla (\Phi), \vec{v}) + \rho \frac{\gamma D}{\rho} - \rho \frac{S}{\rho},
\]

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

The Poisson equation can be written as:

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

where \( p \) is gas pressure, \( \rho_i \) is density of \( i \)-th species, \( s_i \) is speed of formation of \( i \)-th species, \( \rho \) is density of gas mixture, \( n \) is density collisionless component, \( \vec{u} \) is speed gas component, \( \vec{v} \) is speed collisionless component, \( \rho E \) is density of total mechanical gas energy, \( \rho W_{ij} \) is density of total mechanical collisionless components energy, \( \Phi \) is gravitational potential, \( \varepsilon \) is density of internal energy of gas, \( S \) is entropy, \( \gamma \) is adiabatic index, \( \Pi_{ij} \) is a tensor of dispersion of speeds collisionless components, \( S \) is the speed of formation of supernova stars, \( D \) is star formation speed, \( \Lambda \) is function of Compton cooling, \( \Gamma \) is function of heating from explosion of supernova stars.
2.2. Star Formation and Supernova Feedback

The supernovae feedback we should use for SNII, SnIa and other stars by stellar wind $S = S_{\text{SNII}} + S_{\text{SnIa}} + S_\ast$. To describe the supernova feedback we should use the initial mass function [10], stellar lifetimes function [11] and nucleosynthes [12]. For each type of stars we determine their share as $R_{\text{II, Ia,} \ast}$ (see details in work [8]). Also, we determine the rate of star formation by the simple formula:

$$S = \rho \times (R_{\text{SNII}} + R_{\text{SnIa}} + R_\ast)$$

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

$$\Gamma = 10^{51} \times (R_{\text{SNII}} + R_{\text{SnIa}}) \times M_\odot \times V^{-1}$$

We take the rate of star formation $D$ from work [9].

2.3. Cooling and Heating Functions

Chemistry makes the contribution to the cooling and heating functions. We described it in the previous subsection, as well as supernovae feedback. Further, we consider other sources of cooling/heating.

We 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. One can find the collision frequency and the corresponding cooling function in the work [13].

(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. One can find the cooling function in the paper [14].

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

(i) Cosmic ray heating. The process of ionization of hydrogen and helium atoms [15].

(ii) Photoelectric heating from small dust grains [16].

2.4. Supermassive Black Holes

In recent years, many important results have been obtained in the study of the physics of supernovae, the remnants of their explosion and their feedback on more massive structures. So was proved that dwarf galaxies couldn’t be the place of birth of supermassive black holes [17], which in turn is connected with limits of a stars masses in such galaxies. Due to this, given that our main interest further is dwarf galaxies, we won’t introduce the supermassive black holes model in the mathematical model in the near future. Let us stick with its inclusion in the collisionless model.

3. The Chemistry

Let us consider formaldehyde formation in form of sequence of two chemical reactions networks: molecular hydrogen formation and formaldehyde formation from molecular hydrogen with known concentrations proportion $n_{\text{H}_2} : n_{\text{CO}} \approx 6000$ [18]. We divide the description into two parts: one for molecular hydrogen formation and one for formaldehyde formation. Then we combine both solutions and write the analytical expression for a change of formaldehyde concentration using a constant ratio of formaldehyde to molecular hydrogen. We understand that in each particular galaxy this ratio may not be true. However, such ratio between compounds is typical for protoplanetary disks [19]. This means that the ratio is highly common and we can use it.
3.1. Molecular Hydrogen Formation
Hydrogen molecules in intergalactic space are formed on a surface of particles and dissociate space radiation. Assuming that density of a gas is proportional to density of particles concentration of molecular hydrogen [20], due to good mixing of particles and gas in our model, we can write it as:

\[
\frac{dn_{H_2}}{dt} = R_{gr}(T)n_H(n_H + 2n_{H_2}) - (\xi_H + \xi_{diss}(N_{H_2}, A_V)) n_{H_2},
\]

where \(n_{H_2}\) and \(n_H\) are concentrations of molecular and atomic hydrogen, \(N_{H_2}\) is the column density of molecular hydrogen. We set speed of formation of molecular hydrogen on dust by function [21] of \(R_{gr}(T) = 2.2 \times 10^{-18} S \sqrt{T} \ s^{-1}\), where \(S = 0.3\) is efficiency of formation of molecular hydrogen on dust [22]. Let us set speed of ionization of hydrogen by the space beams by function [23, 24] \(\xi_H = 6 \times 10^{-18} \ s^{-1}\), where \(A_e\) is extinction [25]. Photodissociation rate in the form of [26] \(\xi_{diss}(N_{H_2}, A_V) = \xi_{diss}(0)f_{\text{shield}}(N_{H_2})f_{\text{dust}}(A_V)\), where \(\xi_{diss}(0) = 3.3 \times 1.7 \times 10^{-11} \ s^{-1}\) is unshielded photodissociation rate [27], \(f_{\text{dust}}(A_V) = \exp(-\tau_{d,1000}(A_V))\) is absorption rate on dust [26], where \(\tau_{d,1000}(A_V) = 3.74A_V = 10^{-21}(N_H + N_{H_2}) - \) optical depth on dust particles on wavelength \(\lambda = A1000\), where \(N_H\) and \(N_{H_2}\) - column density. We approximate the function of the coefficient of self-defense as follows [26]:

\[
f_{\text{shield}}(N_{H_2}) = \frac{0.965}{(1 + x/b_5)^2} + \frac{0.035}{\sqrt{1 + x}} \exp(-8.5 \times 10^{-4} \sqrt{1 + x}),
\]

where \(x = N_{H_2}/5 \times 10^{10} \ m^2, \ b_5 = b/10^5 \ m/s\), where \(b\) is the parameter of Doppler expansion.

After calculation of molecular hydrogen concentration \(n_{H_2}\), we define the adiabatic index [28]:

\[
\gamma = \frac{5n_H + 7n_{H_2}}{3n_H + 5n_{H_2}}.
\]

3.2. Formaldehyde Formation
We use the work [29] to describe the formaldehyde formation from molecular hydrogen and carbon monoxide \(H_2 + CO \rightarrow H_2CO\). Differential form of formaldehyde formation is as follows:

\[
\frac{dn_{H_2CO}}{dt} = k_Fn_{H_2}n_{CO},
\]

where \(k_F\) is a reaction rate, which is written in Arrhenius form:

\[
k_F = 1.711693 \times 10^{13} \left(\frac{T}{300}\right)^{0.97} \exp\left\{-\frac{-336.4632}{RT}\right\},
\]

where \(T\) is temperature and \(R\) is ideal gas constant.

3.3. Analytical Solution of Formaldehyde Formation
To find analytical solution of the formaldehyde formation let us designate \(m = n_{H_2}\) and \(n = n_{H_2CO}\), taking into account that \(n_H + 2n_{H_2} = M \equiv \text{const}\) and entering symbols:

\[
A = R_{gr}(T) \times M^2, \quad B = R_{gr}(T) \times M - (\xi_H + \xi_{diss}(N_{H_2}, A_V)), \quad C = 6000 \times k_F,
\]

we obtain the following ordinary differential equations:

\[
\frac{dn}{dt} = Cm^2, \quad \frac{dm}{dt} = A - Bm.
\]
For simplicity, let us assume that there is no molecular hydrogen and formaldehyde, that is \( n(0) = m(0) = 0 \), then:

\[
n_{H_2CO}(t) = \frac{A^2 C}{B^3} \times \left( \frac{\exp^2(Bt)}{2} - 2\exp(Bt) + \frac{2t + 3}{2} \right).
\]

In simulation, we use the last solution written in analytical form.

4. The Numerical Method
To solve the hydrodynamic equations, we use a combination of the HLL method with a piecewise parabolic representation of the solution [30, 31]. To solve the Poisson equation, we use a fast Fourier transform method.

4.1. Hydrodynamical Solver
We can write equations for describing the gas and stellar components without taking into account the right-hand side in a single vector form:

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

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

\[
F_{HLL} = \lambda_R F(-\lambda_L \tau) - \lambda_L F(\lambda_R \tau) + \lambda_R \lambda_L (U(-\lambda_L \tau) - U(\lambda_R \tau))
\]

\[
\lambda_L = \min \left( 0; u_L - \gamma \sqrt{\gamma S L \rho_L^{\gamma-1}} \right)
\]

\[
\lambda_R = \max \left( 0; u_R + \gamma \sqrt{\gamma S R \rho_R^{\gamma-1}} \right)
\]

We use equation described in the work [30] to integrate over the parabolas.

4.2. Poisson Solver
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 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 consists 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. We present the resulting density as a superposition of eigenfunctions of the Laplace operator:

\[
\rho_{i,k,l} + n_{i,k,l} = \sum_{jmn} \sigma_{jmn} \exp \left( \frac{\pi i j}{I} + \frac{i \pi k m}{K} + \frac{i \pi l n}{L} \right)
\]

where \( I, K, L \) - the number of cells in each coordinate, \( i \) - imaginary unit. For this, we use fast Fourier transform.
(iii) Solution of the Poisson equation in harmonic space using a fairly simple formula for calculating the amplitudes of the potential harmonics is:

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

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

4.3. Regularization of the solution

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

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

In the other area, we use an adjustment to guarantee non-decreasing entropy:

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

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

5. The Parallel Architecture

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 an 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. On each core, we use vectorization of calculations using AVX-512. We also used a similar approach in the first version of the program code AstroPhi [32] taking into account the use of offload mode.

5.1. Implementation of Vector Operations

In this subsection, we describe the major instructions that we use to implement the method. One can find the full version of the code at the library of the journal, so we will focus only on the declarative description.

- **avx512_vector = _mm512_set1_pd(scalar);**
  Sets elements of the vector to equal scalar value.

- **avx512_vector = _mm512_load_pd(address);**
  loading of 8 double-precision values from the address to the vector.

- **avx512_vector = _mm512_mul_pd(avx512_vec, avx512_vec);**
  multiplication of vectors.

- **avx512_vector = _mm512_add_pd(avx512_vec, avx512_vec);**
  addition of vectors.
• `avx512_vector = _mm512_sub_pd (avx512_vec, avx512_vec);`
  subtraction of vectors.
• `_mm512_stream_pd (address, avx512_vec);`
  writing the vector into memory.

The above instructions are sufficient to implement the HLL method of solving the hydrodynamical equations.

5.2. Code analysis
For the manual performance analysis of the code, we use the problem of a breakdown of discontinuity on the spatial grid $1024 \times 128^2$. We use OpenMP parameters, data alignment and compiler arguments which we considered earlier. For the analysis, we use the infrastructure of Siberian Supercomputer Center NKS-1P (Novosibirsk, Intel Xeon Phi 7290). Maximum performance achieved on Intel Xeon Phi 7290 with 64 threads is 205 GFLOPS. Using 16 Intel Xeon Phi 7290 accelerators we reach 98% scalability.

After these improvements, we achieve 190 GFLOPS performance and 0.3 FLOP/byte arithmetic intensity with 100% mask utilization and 573 GB/s memory bandwidth. This corresponds to manually calculated performance.

6. The Numerical Simulation of Galaxies Collision
We use spheric-symmetric hydrodynamic equilibrium solution:

\[
\begin{align*}
\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d\phi}{dr} \right) &= 4\pi \xi \\
-\frac{d\psi}{dr} - \xi \frac{d\phi}{dr} &= 0
\end{align*}
\]

where $\xi$ – density profile, $\phi$ – gravity profile and $\psi$ – pressure profile. For our simulation we use density profile:

\[
\xi(r) = \begin{cases} 
2r^3 - 3r^2 + 1 & r \leq 1 \\
0 & r > 1
\end{cases}
\]

then gravity profile is:

\[
\phi(r) = \begin{cases} 
\frac{4\pi}{15} r^5 - \frac{3\pi}{5} r^4 + \frac{2\pi}{3} r^2 - \frac{3\pi}{5} & r \leq 1 \\
-\frac{4\pi}{15} & r > 1
\end{cases}
\]

and pressure is:

\[
\psi(r) = \begin{cases} 
-\frac{\pi}{3} r^8 + \frac{44\pi}{35} r^7 - \frac{6\pi}{5} r^6 - \frac{4\pi}{5} r^5 + \frac{8\pi}{5} r^4 - \frac{2\pi}{3} r^2 + \frac{\pi}{7} & r \leq 1 \\
0 & r > 1
\end{cases}
\]

and mass $\mu$ is:

\[
\mu = 4\pi \int r^2 \xi(r) dr = \frac{4\pi}{15}
\]

We use mass ratio

\[
\frac{M_{gas}}{M_{stars+DM}} = \frac{m}{k}
\]

Then profile is:

\[
\rho(r) = m \times \xi(r), \quad n(r) = k \times \xi(r), \\
p(r) = m(m + k) \times \psi(r), \quad \Pi(r) = k(m + k) \times \psi(r),
\]
Figure 1. The column density of the baryon matter (a), gas (b), stars (c), molecular hydrogen (d), formaldehyde (e) in $M_\odot pc^{-2}$ at the moment of time 200 Myr, and star formation rate (f) in $M_\odot pc^{-2} Myr^{-1}$, are in the picture.
\Phi + \Phi_0 = (m + k) \times \phi(r).

The picture 1 shows the results of galaxies collision simulation. The bulk of molecular hydrogen is formed in the shock wave near the scattering stellar components. Let us note, that high mass of the stars in the center of the area doesn’t lead to hydrogen formation. Though the temperature required for the active passage of molecular hydrogen formation reactions is maintained. Let us also note, that the high star formation rate is in the areas with low molecular hydrogen and formaldehyde concentrations. Formaldehyde molecules distribution generally corresponds to molecular hydrogen position but is more accentuated in the shock waves centers, where the maximum temperature is reached. Apparently, the only key factor of complex compounds formation is a high temperature of shock waves. That generally corresponds to observational data and conclusions by them. In the numerical experiment, we use a computational area [64 kpc]\(^3\) and computational grid 256\(^3\). There is 2000 time-steps. We use one node of the NKS-30T cluster of Siberian Supercomputer Center for calculations.

7. Conclusion
We presented the new hydrodynamical code for modeling of the galaxies collision on supercomputers equipped with Intel Xeon Phi in the paper. 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 is in the basis of the mathematical model of interacting galaxies. We described the structure of the parallel numerical method for solving the hydrodynamics equations. We showed The scenarios of interacting galaxies. We described the chemistry in interacting galaxies.

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