A NEW CODE FOR NUMERICAL SIMULATION OF MHD ASTROPHYSICAL FLOWS WITH CHEMISTRY

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ABSTRACT

The new code for numerical simulation of magnetic hydrodynamical astrophysical flows with consideration of chemical reactions is given in the paper. At the heart of the code — the new original low-dissipation numerical method based on a combination of operator splitting approach and piecewise-parabolic method on the local stencil. The details of the numerical method are described; the main tests and the scheme of parallel implementation are shown. The chemodynamics of the hydrogen while the turbulent formation of molecular clouds is modeled.

Subject headings: MHD — methods:numerical — molecular clouds — galaxy cluster — interstellar wind

1. INTRODUCTION

Magnetic field plays a key role in formation and dynamics of astrophysical objects. Thus, on cosmological scales the influence of weak magnetic field, with order $\mu G$, on the dynamics of hydrodynamical instabilities and ram-pressure mechanism in galactic clusters (Bruggen 2013) was studied; primarily radial orientation of the magnetic field in Virgo cluster outside the central area was defined (Pfrommer & Duras 2010), and comparison of magnetic field with radio observation was carried out (Xu et al. 2012). The structure of magnetic field in spiral arms of the M51 galaxy was investigated (Fletcher et al. 2011), and the evolution of the disk galaxy with consideration of influence of magnetic field was modeled (Pakmor & Springel 2013). The consideration of the influence of magnetic field plays an important role in the evolution of interstellar turbulent flows where the magnetic field is sufficiently strong (Perez & Boldyrev 2010; Mason et al. 2011). In the problems of evolution of MHD instabilities the power spectrum (Beresnyak 2014), sub-alfvenic flows (McKee et al. 2010), and starburst rate (Federrath & Klessen 2012) were studied, and the comparison of different codes on the problem of supersonic turbulence was made (Kritsuk et al. 2011). In the problems connected with the stellar wind, the MHD simulation is necessary too. Thus, the turbulence in stellar wind was investigated (Galtier & Buchlin 2007), one-dimensional MHD model of interaction of stellar wind with 67P/Churyumov-Gerasimenko comet (Mendis & Horanyi 2014), Halley comet (Ogino et al. 1988), and also gas planet (Johnstone et al. 2015). Shematovich et al. (2014) was built. In addition, the similar problems of interaction between stellar wind and stars (Villaver et al. 2012) are worth noting.

Besides earlier classical (AMR and SPH) approaches (see the methods and codes overview in (Kulikov 2014; Kulikov et al. 2015a) and in classical monography (Kulikovskii et al. 2001)) a lot of new original numerical methods and codes for astrophysical MHD flows simulations were made for the last decade. For example, in CosmoMHD code (Li et al. 2008) based on TVD-ES approach MHD equations are solved in extended form with additional equations for internal energy and entropy. Such approach allows better simulations of flows with large Mach numbers (Balsara & Spicer 1999a) because of entropy conservation law. However, the possibility of growth of entropy within shock waves is an opened issue, because the equation for entropy is formulated as inequality (Godunov & Kulikov 2014) and, in fact, doesn’t use in computations so as an equation for internal energy, except, perhaps, the areas with low-density (Vshivkov et al. 2011b). The GOEMHD3 (Skala et al. 2015) code, based on the combination of a leap-frog, Lax and DuFort-Frankel finite-differential schemes for a non-conservative form of MHD equations, was developed for simulation of MHD flows with large Reynolds number. Nevertheless, such formulation had allowed reproducing solution with Reynolds number $10^{10}$ good enough. Also, codes based on Godunov type solvers with high order accuracy such as Athena (Stone et al. 2008). Fish (Kappe1 et al. 2011), MPI-AMRVAC (Porth et al. 2014), Pluto (Mignone et al. 2011), and code based on piecewise-parabolic method on local stencil (Popov & Ustyugov 2007, 2008) are worth noting. TVD reconstruction of numerical solution is used in all of them that is naturally in methods with high order accuracy. Besides, the Flux-CT scheme (Balsara & Spicer 1999a) based on Stokes theorem is used to to comply with the term $\nabla \times \vec{B} = 0$, that is more efficient than projection schemes (Brackbill & Barnes 1980) used in couple of codes (Springel 2010).

The new low-dissipation numerical scheme for solving equations of magnetic gas dynamics with consideration of chemical processes and its software implementation...
are presented in the paper. The numerical method is based on hybrid method developed earlier with combination of operator splitting approach and Godunov method in its basis (Tutukov et al. 2011; Vshivkov et al. 2009, 2011a, b; Godunov & Kulikov 2014; Kulikov 2014; Kulikov et al. 2015a, b; Kulikov & Vorobyov 2016; Protasov & Kulikov 2015; Protasov et al. 2016). The piecewise-parabolic method on local stencil is used in all stages of the scheme to get low dissipation of the solution. The special algorithm for building the local parabola had allowed us to fully eliminate the using of TVD reconstructions of the numerical solution in the region of discontinuous solutions. We specifically do not claim the new method as a method of high order accuracy, because this term is not fully formulated in a case of discontinuous solutions (Godunov et al. 2011). In the first section, the numerical method is defined, and its software implementation is briefly described. In the second section, the one- and two-dimensional tests are shown. The third section is devoted to simulation of 3D MHD flows.

2. NUMERICAL METHOD DESCRIPTION

In this paper, we will only consider the MHD flows, and the model problems will be considered just in MHD approximation. Thus, the system of equations of gravitational multicomponent magnetic gas dynamics in 3D cartesian coordinates taking into account the function of heating and cooling is used:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} &+ \nabla \cdot (\rho \mathbf{v}) = 0 \\
\frac{\partial \rho_i}{\partial t} &+ \nabla \cdot (\rho_i \mathbf{v}) = \mathcal{S}_i \\
\frac{\partial \rho \mathbf{v}}{\partial t} &+ \nabla \cdot (\rho \mathbf{v} \mathbf{v} - \mathbf{B} \nabla \cdot \mathbf{B}) = - \nabla p^* - \rho \nabla \Phi \\
\frac{\partial \rho E}{\partial t} &+ \nabla \cdot (\rho E \mathbf{v} + p^* \mathbf{v} - \mathbf{B} (\nabla \cdot \mathbf{B})) = -(\rho \mathbf{v} \nabla \Phi) + \Gamma - \Lambda \\
\frac{\partial \rho \varepsilon}{\partial t} &+ \nabla \cdot (\rho \varepsilon \mathbf{v}) = - (\gamma - 1) \rho \varepsilon \nabla \cdot \mathbf{v} + \Gamma - \Lambda \\
\frac{\partial \mathbf{B}}{\partial t} &- \nabla \times (\mathbf{v} \times \mathbf{B}) = 4\pi G \rho \\
\nabla \cdot \mathbf{B} & = 0
\end{align*}
\]

the condition of non-divergency of magnetic field

\[
\nabla \cdot \mathbf{B} = 0
\]

where \(\rho = \sum \rho_i\) — density, \(\rho_i\) — density of each component of the gaseous mixture, \(\mathcal{S}_i\) — formation rate of \(i\)-th component of the mixture, \(\mathbf{v}\) — velocity, \(\mathbf{B}\) — magnetic field, \(p = \rho \varepsilon (\gamma - 1)\) — pressure, \(\rho \varepsilon\) — internal energy, \(p^* = p + \mathbf{B}^2/2\) — full pressure, \(\gamma -\) adiabatic index, \(\rho E = \rho \varepsilon + \rho \mathbf{v}^2/2 + \mathbf{B}^2/2\) — full mechanical energy, \(\Phi\) — gravitational potential, \(\Gamma\) — heating function, \(\Lambda\) — cooling function, \(G\) — gravitational constant.

The method of solving equations of gravitational multicomponent magnetic gas dynamics is based on a combination of operator splitting approach and Godunov method with using the piecewise-parabolic method on the local stencil. It consists of the following stages:

1. eulerian stage, at which the equations for density, impulse, full and internal energy are solved without consideration of advective terms and functions of heating and cooling, but with consideration of work of gravitational force;

2. recomputation of magnetic field with conservation of condition \(\nabla \cdot \mathbf{B} = 0\) with using of Flux-CT scheme;

3. lagrangian stage, at which the advection of density, momentum, full, and internal energy happens;

4. solving of homogeneous differential equations in each cell of computational domain to compute concentration of gas mixture;

5. consideration of subcell processes of cooling/heating;

6. regularization of numerical solution;

7. solving of Poisson equation to compute gravitational potential.

Before proceeding to the detailed description of each stage let us describe two procedures, on which the eulerian and lagrangian stages are based – the procedure of building the local parabolas, which will be used in solution of the Riemann problem at each stage; and the procedure of using the fourth-order Runge-Kutta method that used on the eulerian and lagrangian stages separately.

2.1. Procedure of building of the local parabolas

For definiteness we will construct piecewise-parabolic function of particular parameter \(q(x)\) on the regular grid with step \(h\) in the interval \([x_{i-1/2}, x_{i+1/2}].\) In general, parabola could be written as:

\[
q(x) = q_i^L + \xi \left( \Delta q_i + q_i^{(6)} (1 - \xi) \right)
\]

where \(q_i\) — value in the center of cell, \(\xi = (x - x_{i-1/2})/h^{-1},\) \(\Delta q_i = q_i^L - q_i^R\) and \(q_i^{(6)} = 6(q_i - 1/2(q_i^L + q_i^R))\) while maintaining conservatism, that is:

\[
q_i = h^{-1} \int_{x_{i-1/2}}^{x_{i+1/2}} q(x) dx
\]

Let us give the detailed procedure of building of the parabola and parameters \(q_i^L, q_i^L, \Delta q_i, q_i^R.\) To construct the values \(q_i^R = q_i^{L+1}\) and \(q_i^{(6)} = 6(q_i - 1/2(q_i^L + q_i^R))\) fourth-order interpolation function will be used:

\[
q_i^{L+1/2} = 1/2(q_i + q_{i+1}) - 1/6(\delta q_{i+1} - \delta q_i)
\]

where \(\delta q_i = 1/2(q_{i+1} - q_{i-1}).\) Further, we describe the algorithm of building the local parabola. The input is the values in centers of cells \(q_i.\) The output of the algorithm is all of the parameters of piecewise-parabolic functions in each interval \([x_{i-1/2}, x_{i+1/2}].\)

**Step 1.** At the first step the values \(\delta q_i = 1/2(q_{i+1} - q_{i-1})\) are constructed. To do this we need to know only
nearby cells \( q_{i+1}, q_{i-1} \). To eliminate the extrema of functions the modification of the last formula for \( \delta q_i \) is used as follows:

\[
\delta q_i = \begin{cases} 
\min(|\delta q_i|, 2|q_{i+1} - q_i|, 2|q_i - q_{i-1}|) \text{sign}(\delta q_i), \\
0, (q_{i+1} - q_i)(q_i - q_{i-1}) > 0 \\
0, (q_{i+1} - q_i)(q_i - q_{i-1}) \leq 0 
\end{cases}
\]

The exchange of the one layer of overlapping should be done with using of MPI in the case of a parallel implementation on the architectures with distributed memory. Then, the values on the borders are recomputed with using of the fourth-order interpolant:

\[
q_i^R = q_{i+1}/2 = 1/2(q_i + q_{i+1}) - 1/6(\delta_m q_{i+1} - \delta_m q_i)
\]

**Step 2.** At the second step of the algorithm the local parabola is constructed with using of the following formula:

\[
\Delta q_i = q_i^L - q_i^R \\
q_i^{(6)} = 6(q_i - 1/2(q_i^L + q_i^R))
\]

The values on the borders \( q_i^L, q_i^R \) in case of non-monotonic local parabola (it could happen in discontinuities) are reconstructed according to the formulas:

\[
q_i^L = q_i, q_i^R = q_i, (q_i^L - q_i)(q_i - q_i^R) \leq 0 \\
q_i^L = 3q_i - 2q_i^R, \Delta q_i^{(6)} > (\Delta q_i)^2 \\
q_i^R = 3q_i - 2q_i^L, \Delta q_i^{(6)} < - (\Delta q_i)^2
\]

Thus, the boundary values satisfy the conditions of monotonicity.

**Step 3.** At the third step the parabola parameters are reconstructed with consideration of new values in boundary cells:

\[
\Delta q_i = q_i^L - q_i^R \\
q_i^{(6)} = 6(q_i - 1/2(q_i^L + q_i^R))
\]

It is worth noting, that parabolas could have a discontinuity on the borders of cells, that leads to the need of solving of the Riemann problem for parabolas in case of using of classical piecewise-parabolic method (PPM). In our case the local parabolas are used as a part of the Riemann problem.

**Step 4.** At the fourth step additional monotinization of parabola is done. If we are in the region of discontinuity of the function, then the additional amendments are made:

\[
q_i^{L,+} = q_i - \frac{1}{4} \delta_m q_i \\
q_i^{R,+} = q_i + \frac{1}{4} \delta_m q_i
\]

Additional criteria is introduced:

\[
\eta = -h^2 \frac{\delta^2 q_{i+1} - \delta^2 q_{i-1}}{q_{i+1} - q_{i-1}}
\]

If one of the follow inf conditions is satisfied:

\[
|q_{i+1} - q_{i-1}| - \min(|q_{i+1}|, |q_{i-1}|, |q_{i+1} + q_{i-1}|) \leq 0 \\
q_{i+1} + q_{i-1} > 0
\]

the value of the criteria \( \eta \) is set to zero. The weight of values \( q_i^{L,+}, q_i^{R,+} \) in the computational scheme is defined by the formula:

\[
h = \max(\min(20(\eta - 0.05), 1), 0)
\]

Final values of the flows are computed by the formulas:

\[
q_i^{L,FINAL} = (1-h)q_i^{L,+} + h q_i^L \\
q_i^{R,FINAL} = (1-h)q_i^{R,+} + h q_i^R
\]

The last two values are used to determ the quantities \( q_i^L, q_i^R \). Such additional monotonicity is done for all magneto-hydrodynamics quantities in contrast to classical procedure in (Collela & Woodward 1984), and also slightly different ways to compute the gradient of the solution were experimentally found.

**Step 5.** At the fifth step the final reconstruction of the parabola with consideration of new values on the borders of the cell is made:

\[
\Delta q_i = q_i^L - q_i^R \\
q_i^{(6)} = 6(q_i - 1/2(q_i^L + q_i^R))
\]

As a result the local parabola in every cell \([x_{i-1/2}, x_{i+1/2}]\) is computed. Notice, that monotonicity of the numerical solution have a place only at the stage of building of the local parabola, which is used for solving the Riemann problem at each stage.

2.2. Runge-Kutta time integration scheme

Using the finite-volume approximation of eulerian and lagrangian stages, described further, the numerical scheme could be written in form of ordinary differential equation as follows:

\[
\frac{dQ}{dt} = \mathcal{R}
\]

where \( Q \) – magnetic-hydrodynamics parameters, \( \mathcal{R} \) – finite-volume approximation of each stage. In this case the Runge-Kutta scheme for approximation of the derivations by time will be used to compute the solution at each stage:

\[
Q^{(n+1/3)} = Q^{(n)} + \tau \mathcal{R}^{(n)} \\
Q^{(n+2/3)} = \frac{3}{4} Q^{(n)} + \frac{1}{4} Q^{(n+1/3)} + \frac{\tau}{4} \mathcal{R}^{(n+1/3)} \\
Q^{(n+1)} = \frac{1}{3} Q^{(n)} + \frac{2}{3} Q^{(n+2/3)} + \frac{2\tau}{3} \mathcal{R}^{(n+2/3)}
\]

where \( \mathcal{R}^{(i)} \) – the solution at each stage on the \( i \)-th layer of time, \( \mathcal{R}^{(i)} \) – finite-volume approximation of equations on the \( i \)-th layer of time.

2.3. Compliance with the Courant-Friedrichs-Lewy condition

To choose the time step \( \tau \) the speed of sound \( c = \sqrt{\frac{\gamma p}{\rho}} \), alflowen speed of sound \( c_a = \sqrt{\frac{F}{\gamma \rho}} \), fast \( c_f \) and slow \( c_s \) magnetic speeds:

\[
c_f = \sqrt{\frac{(c^2 + b^2) + \sqrt{(c^2 + b^2)^2 - 4c^2c_s^2}}{2}} \\
c_s = \sqrt{\frac{(c^2 + b^2) - \sqrt{(c^2 + b^2)^2 - 4c^2c_a^2}}{2}}
\]
where \( b = \sqrt{B_x^2 + B_y^2 + B_z^2} \) are determined in each cell. Then the time step is computed according to the equation:

\[
\tau = \min \left( \frac{CFL \times b}{v + b + c + c_a + c_s + c_f} \right)
\]

where \( v = \sqrt{v_x^2 + v_y^2 + v_z^2} \) – speed, \( h \) – length of the edge of a cell, \( CFL = 0.2 \) – the Courant-Friedrichs-Lewy number.

2.4. Eulerian stage

At the eulerian stage of the scheme the linearized Godunov method is used. Gravitational force is calculated using of central differential scheme because of smoothness of gravitational potential. The Riemann problem with piecewise-parabolic initial conditions in all directions is formulated to compute magnetic hydrodynamic flows on the borders of each computational cell:

\[
\frac{\partial q}{\partial t} + B \frac{\partial q}{\partial x} = 0
\]

In case of MHD equations for eulerian stage the vector \( q = (v_x, v_y, v_z, B_y, B_z, p)^T \), and the matrix \( B \) on each border of cells is written as follows:

\[
B = \begin{pmatrix}
0 & 0 & 0 & B_y & B_z & \frac{1}{\rho} \\
0 & 0 & 0 & -\frac{B_y}{\rho} & 0 & 0 \\
0 & 0 & 0 & 0 & -\frac{B_z}{\rho} & 0 \\
B_y & -B_x & 0 & 0 & 0 & 0 \\
B_z & 0 & -B_x & 0 & 0 & 0 \\
\gamma p & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\]

To average magnetic-hydrodynamics values from left (L) and right (R) cells on the border between them the following equations are used:

\[
\rho = \frac{\sqrt{\rho L \rho L} + \sqrt{\rho R \rho R}}{\sqrt{\rho L^2} + \sqrt{\rho R^2}}
\]

\[
v_{[x,y,z]} = \frac{\sqrt{\rho L v_{L[x,y,z]}^3} + \sqrt{\rho R v_{R[x,y,z]}^3}}{\sqrt{\rho L^2} + \sqrt{\rho R^2}}
\]

\[
B_{[x,y,z]} = \frac{\sqrt{\rho L B_{L[x,y,z]}^3} + \sqrt{\rho R B_{R[x,y,z]}^3}}{\sqrt{\rho L^2} + \sqrt{\rho R^2}}
\]

after that the speed of sound \( c \), alfvénic speed of sound \( c_a \), fast \( c_f \) and slow \( c_s \) magnetic speed could be calculated by the equations form the previous section. For the eigenvalue-decomposition matrix \( B \) the definition of the following parameters should be extended:

\[
(\alpha_f, \alpha_s) = \begin{cases}
(\sqrt{c_f^2 - c_s^2}, \sqrt{c_f^2 - c_s^2}) & B_y^2 + B_z^2 > 0, \gamma p \neq B_x^2 \\
(1, \sqrt{c_f^2 - c_s^2}) & B_y^2 + B_z^2 = 0, \gamma p = B_x^2 
\end{cases}
\]

\[
(\beta_f, \beta_s) = \begin{cases}
\left(\frac{B_y}{B_x^2 + B_z^2}, \frac{B_z}{B_x^2 + B_z^2}\right) & B_y^2 + B_z^2 > 0 \\
\left(\frac{1}{\sqrt{c_f^2 - c_s^2}}, \sqrt{c_f^2 - c_s^2}\right) & B_y^2 + B_z^2 = 0
\end{cases}
\]

The matrix \( B \) could be written as eigenvalue-decomposition \( B = RL \), where \( R \) and \( L \) are mutually orthogonal matrices \( RL = LR = I \) of right and left eigenvectors (their form is given in appendix). \( \Omega \) is a diagonal matrix with eigenvalues:

\[
\lambda_1 = c_f \quad \lambda_2 = -c_f \quad \lambda_3 = c_s \quad \lambda_4 = -c_s \\
\lambda_5 = c_a \quad \lambda_6 = -c_a
\]

Replacing \( s = Lq \) we get the system

\[
\frac{\partial s}{\partial t} + \Omega \frac{\partial s}{\partial x} = 0
\]

which could be solved analytically but with the consideration that initial conditions \( s^0 \) for this problem is a piecewise-parabolic functions. Thus, the solution of Riemann problem for the last system of equations could be formulated in form:

\[
s_1 = s_1^0 (c_f \tau) \quad s_2 = s_2^0 (c_f \tau) \quad s_3 = s_3^0 (c_s \tau) \\
s_4 = s_4^0 (c_s \tau) \quad s_5 = s_5^0 (c_a \tau) \quad s_6 = s_6^0 (c_a \tau)
\]

Depending on the sign of eigenvalue the integration should be made by the left or the right parabola. Using the notations from section (2.1) solution could be written as follows:

\[
q(-\nu t) = q_i^R - \frac{\nu t}{2h} \left( \Delta q_i - q_i^0 \left( 1 - 2\nu t \frac{v}{3h} \right) \right)
\]

\[
q(\nu t) = q_i^L + \frac{\nu t}{2h} \left( \Delta q_i + q_i^0 \left( 1 - 2\nu t \frac{v}{3h} \right) \right)
\]

where \( \nu \) – modulus of the eigenvalue, \( i \) – the number of cell depending on the consideration of the left or the right parabola. After the Riemann problem is solved for the vector \( s \), using the replacement \( q = R s \) the solution of the Riemann problem is calculated \( V_x, V_y, V_z, B_y, B_z, P \), that is used in the finite-volume approximation further (their final form is given in appendix).

2.5. Satisfying the condition \( \nabla \cdot (B) = 0 \)

To satisfy the condition \( \nabla \cdot (B) = 0 \) the Flux-CT scheme \( \text{(Balsara & Spicer 1999b)} \) based on Stokes theorem was used:

\[
\frac{\partial B}{\partial t} = \nabla \times (v \times B)
\]

We will use follow schemas of cell \( (i, k, l) \) (see. fig. 1) and condition \( h_x = h_y = h_z = h \). The magnetic field vector will define on border of cells:

\[
B_n^{i+1/2,k,l} = B_{x,i+1/2,k,l}^n
\]
where \( C_i \) – speed of construction of \( i \)-th component, \( D_i \) – speed of destruction of \( i \)-th component. To solve such differential equations the scheme of inverse differentiation is used:

\[
n_{i}^{t+\tau} = n_i^t + \tau C_i - D_i n_i^t
\]

We understand that it is, possibly, not the best way and, for example, using the code KROME (Grassi et al. 2014) is more efficient but a similar approach was successfully used in works (Glover & Mac Low 2007; Anninos et al. 1997).

2.8. Subgrid physics

To consider the subgrid physics the following equations are solved:

\[
\begin{align*}
\frac{\partial \rho E}{\partial t} &= \Gamma - \Lambda \\
\frac{\partial \rho \varepsilon}{\partial t} &= \Gamma - \Lambda
\end{align*}
\]

in each cell with using of Euler method for solving the ODE. There is no matter to use complex way of approximation of Runge-Kutta type because the values of heating and cooling functions are constant while the time step in each cell of the computational domain.

2.9. Regularization of numerical solution

At the stage of regularization of the solution the correction of speed on the gas-vacuum interface, where the condition \(( E - \varepsilon^2/2 - B^2/2 \rho)/E \geq 10^{-3}\) is satisfied, is done with using of approach similar to the one described in (Vshivkov et al. 2011b):

\[
|v| = \sqrt{2 \rho E - \rho \varepsilon - B^2/2 - \rho}
\]

in the rest area the correction, that guarantees non-decreasing of entropy, like in work (Godunov & Kulikov 2014) is made:

\[
\rho \varepsilon = \rho E - \rho \varepsilon^2/2 - B^2/2
\]

Such modification allows the detailed balance of energies and guarantee non-decreasing of entropy.

2.10. Solution of the Poisson equation

To solve the Poisson equation the 27-point pattern with the following scheme of solution in the harmonic space is used:

\[
\Phi_{jmn} = \frac{2}{3} \pi h^2 \rho_{jmn}
\]

The Fast Fourier Transform is used to make a transition into the harmonic space, that is in finding the transition coefficients. The FFT is in a heart of the method of solving the Poisson equation. To perform it on supercomputers with distributed memory the FFTW library (Frigo & Johnson 2005) was used. The library is based on procedure ALLTOALL, that "transport" 3D array redistributing huge amount of memory between processes. Certainly, it is expensive network operation demanding to eliminate using of the whole algorithm if we have any significant count of processors. Nevertheless, this procedure doesn’t get much time while using of InfiniBand network infrastructure and, apparently, optimized in low network level (Kalinkin et al. 2009).
tion. Also the condition code reproduce formation of shocks and their interactions of the solution near the discontinuity region, and propagate not more than on three cells; there are no oscillations of the solution near the discontinuity region, and also contact discontinuity is reproduced correctly.

2.11. Parallel implementation

The parallel implementation is based on the geometrical decomposition of the computational area with one layer of overlapping of the subregions by using of MPI. The study of scalability of the code was made with using of equipment of SSCC on 1 to 768 of Intel Xeon X5670 cores. The 93 % efficiency was achieved on 768 computational cores (see fig. 2).

3. VERIFICATION WITH 1D AND 2D TESTS

3.1. One dimensional shock tube problem

To verify the method the 1D problem was formulated. The solution of this problem include each type of MHD shocks evolving by both regions separated by contact discontinuity [Barmin et al. 1996]. The problem is being solved in region [0; 1]; initial discontinuity is being set in point \( x_0 = 0.5 \). To the left of the discontinuity the gas parameters are \((\rho, p, v_x, v_y, B_y/\sqrt{4\pi}, B_z/\sqrt{4\pi}) = (0.18405, 0.3541, 3.8964, 0.5361, 2.4866, 2.394, 1.197)\); on the right side parameters of the gas has a more simple form \((\rho, p, v_x, v_y, v_z, B_y/\sqrt{4\pi}, B_z/\sqrt{4\pi}) = (0.1, 0.1, -5.5, 0, 0, 2, 1)\), \( x \)-component of magnetic field \( B_z/\sqrt{4\pi} = 4 \), adiabatic index \( \gamma = 1.4 \). The numerical solution of the problem in the moment \( t = 0.15 \) is shown in figure 3.

Notice, that each shock is reproduced correctly [Barmin et al. 1996]; smearing of MHD shocks is propagated not more than on three cells; there are no oscillations of the solution near the discontinuity region, and also contact discontinuity is reproduced correctly.

3.2. Orszag-Tang Vortex Test

Orszag-Tang Vortex problem [Orszag & Tang 1979] is the most popular model for testing the transition to supersonic turbulence, and it verifies how correctly the code reproduce formation of shocks and their interaction. Also the condition \( \nabla \cdot (\mathbf{B}) = 0 \) could be tested on this problem. In the problem we consider the region \([0; 1]^2\) with periodic border conditions in each direction, that is filled uniformly with density \( \rho = 25/(36\pi) \) ad pressure \( p = 5/(12\pi) \). Initial speed \( v_x = -\sin(2\pi y) \) and \( v_y = \sin(2\pi x) \). Initial magnetic field \( B_x = -B_0 \sin(2\pi y) \) and \( B_y = B_0 \sin(4\pi x) \), where \( B_0 = 1/\sqrt{4\pi} \). Adiabatic index \( \gamma = 5/3 \). Numerical solution of the problem in the moment of time \( t = 0.2 \) is shown in figure 4. Notice, that density field and structure of vector magnetic field are consistent with many results of other authors.

4. SIMULATION OF 3D MHD FLOWS

To verify the numerical method and program implementation in 3D, three problems in MHD statement were studied: the collision of two galaxy clusters with different mass, similar to Bullet cluster collision scenario [Mastropietro & Burkert 2008; Lage & Farrar 2014]; the problem of interaction of molecular cloud and interstellar medium [Villaver et al. 2012]; the problem of evolution of MHD turbulence of an interstellar medium [Ustyugov et al. 2009; Kritsuk et al. 2009] with consid-
The profile of the density is:

\[ \rho(r) \sim 2r^3 - 3r^2 + 1 \]

The value of vertical magnetic field is \( B_0 = 0.05 \mu G \).

The results of simulation are in figures 8 and 9. In the beginning, there is an overrunning of the flow and formation of the shock wave in front of the molecular cloud. Also, significant reconstruction of the magnetic field on the fronts of interaction is visible.

4.3. Chemodynamics of evolution of MHD turbulence of the interstellar medium

The problem of chemodynamics of evolution of MHD turbulence of the interstellar medium was examined in full formulation with consideration of self-gravitation. To do this, the region \( [256 \text{pc}]^3 \) with vertical component of magnetic field, uniform initial concentration of atoms \( n = 5 \text{cm}^{-3} \), initial random perturbation with speed \( v_{rms} = 10 \text{km/s} \), initial value of plasma parameter \( \beta_h = 8\pi \rho_p / B_0^2 = 25 \), initial value of turbulent plasma parameter \( \beta_{turb} = 8\pi \rho_{rms}^2 / B_0^2 = 25 \), and Alfvenic Mach number \( M = 3.52 \), was considered. The following eight reactions, that was also used in work (Glover & Mac Low 2007), was examined.

1. Molecular hydrogen formation (Hollenbach & McKee 1979):
   \[ H + H + \text{grain} \rightarrow H_2 + \text{grain} \]
   which held with speed \( k_1 \) and initiate heating of \( \Gamma_1 \).

2. Molecular hydrogen first dissociation (Lepp & Shull 1983):
   \[ H_2 + H \rightarrow 3H \]
   which held with speed \( k_2 \) and initiate heating of \( \Lambda_2 \).

3. Molecular hydrogen second dissociation (Martin et al. 1998):
   \[ H_2 + H_2 \rightarrow 2H + H_2 \]
   which held with speed \( k_3 \) and initiate cooling of \( \Lambda_3 \).
4. Molecular hydrogen photodissociation (Glover & Mac Low 2007):
   \[ H_2 + \gamma \rightarrow 2H \]
   which held with speed \( k_4 \) and initiate heating of \( \Gamma_4 \).
5. Cosmic Ray ionization (Glover & Mac Low 2007):
   \[ H + c.r. \rightarrow H^+ + e \]
   which held with speed \( k_5 \) and initiate heating of \( \Gamma_5 \).
6. Collision ionization (Abel et al. 1997):
   \[ H + e \rightarrow H^+ + 2e \]
   which held with speed \( k_6 \) and initiate cooling of \( \Lambda_6 \).
7. Radiative recombination (Ferland et al. 1992):
   \[ H^+ + e \rightarrow H + \gamma \]
   which held with speed \( k_7 \) and initiate cooling of \( \Lambda_7 \).
8. EI recombination on grains (Weingartner & Draine 2001):
   \[ H^+ + e + \text{grain} \rightarrow H + \text{grain} \]
   which held with speed \( k_8 \) and initiate cooling of \( \Lambda_8 \).

Each speed of reaction and also an analytical form of the cooling and heating functions are listed in the appendix. Effective adiabatic index was used in the following form:

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

Behaviour of concentration of different forms of hydrogen, which mostly was ionized, and molecular hydrogen was a several thousandth of a percent (see fig. 7), was modeled with using of code ChemPAK (Chernykh et al. 2009) for specific values of temperature \( T = 1000 \) K and \( T = 5000 \) K, and also for specific concentration of atomic neutral hydrogen. In numerical experiment concentrations behaved in a similar way.

The results of the simulation are shown in figure 9. The formation of some small waves of density in the moments \( t = 10 \) and \( t = 14 \) Myr is visible in the figure. However, then the clusterization process is accelerated, that leads to the formation of clouds. Of course, we couldn’t say it is possible to simulate the most known part of Carina Nebula, but, in our opinion, some kind of finger-like formations were obtained during the simulation.

Also dependence of the alfvenic speed on the gas density (see fig. 11 on the left), and dependence of cosine of an angle of collinearity between velocity and vector of magnetic field on the gas density (see fig. 11 on the right). It is clear from the figures, that for alfvenic Mach number the correlation \( M \sim n^2 \) is visible in the figure. However, the most part of the cloud \( n > 10 \text{cm}^{-3} \) is in the over-alfvenic region (see fig. 11 on the left). The reason of emergence of such mode is in magnetic turbulent interstellar medium in trans-alfvenic mode \( M \sim 1 \) with \( n \sim 1 \). With such densities (see fig. 11 on the right) contours of the cosine of an angle of collinearity between velocity and vector of magnetic field forms saddle-like structure, which means that the compression is along force lines of magnetic field. Then, further increase of mass and density of the cloud happening due to the influence of self-gravitation. In its turn, in dense clouds turbulence is just over-alfvenic with Mach number \( M > 100 \).

5. CONCLUSION

In the paper, the new code for numerical simulation of magnetic hydrodynamical astrophysical flows with consideration of chemical reactions is given. New original low-dissipation numerical method, based on a combination of operator-splitting approach and piecewise-parabolic method on a local stencil, for solving equations of magnetic-hydrodynamics is described in details. The scheme of program and results of scalability on classical multiprocessor architectures is given. Numerical method and its program implementation were verified with using of basic problems. Chemodynamics of hydrogen during the process of turbulent formation of molecular clouds was modeled.

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REFERENCES

Abel, T., Anninos, P., Zhang, Y., & Norman, M. 1997, NewA, 2, 181.
Anninos, P., Zhang, Y., Abel, T., & Norman, M. 1997, NewA, 2, 209.
APPENDIX

Matrix of the right \( R \) and left \( L \) eigenvectors in the Riemann problem at the Eulerian stage are:

\[
R^T = \begin{pmatrix}
\alpha \gamma \rho \beta \sigma \delta \eta \mu \nu \\
-\alpha \gamma \rho \beta \sigma \delta \eta \\
0 & -\beta \gamma \rho \sigma \delta \eta \\
0 & -\gamma \rho \sigma \delta \eta
\end{pmatrix}
\]

\[
L = \begin{pmatrix}
\alpha \gamma \rho \beta \sigma \delta \eta \mu \nu \\
-\alpha \gamma \rho \beta \sigma \delta \eta \\
0 & -\beta \gamma \rho \sigma \delta \eta \\
0 & -\gamma \rho \sigma \delta \eta
\end{pmatrix}
\]

APPENDIX

Exact solution of the Riemann problem at the Eulerian stage for \( x \) – longitude component of velocity is written in
the grid with $512^3$ cells was used.

$V_x = \left( \frac{\alpha c \nu}{2c^2} (v_x (c_s \tau) + v_x (-c_s \tau)) \right) + \left( \frac{\alpha \beta \alpha \beta \nu \sigma}{2c^2} (v_y (c_s \tau) + v_y (-c_s \tau) - v_y (c_s \tau) - v_y (-c_s \tau)) \right) + \\
\left( \frac{\alpha \beta \alpha \beta \nu \sigma}{2c^2} (v_z (c_s \tau) + v_z (-c_s \tau) - v_z (c_s \tau) - v_z (-c_s \tau)) \right) + \\
\left( \frac{\alpha \beta \alpha \beta \nu \sigma}{2c^2} (b_y (-c_f \tau) - b_y (c_f \tau)) \right) + \left( \frac{\alpha \beta \alpha \beta \nu \sigma}{2c^2} (b_z (-c_f \tau) - b_z (c_f \tau)) \right) + \\
\left( \frac{\alpha \beta \alpha \beta \nu \sigma}{2c^2} (p (-c_f \tau) - p (c_f \tau)) \right) + \\
\left( \frac{\alpha \beta \alpha \beta \nu \sigma}{2c^2} (b_y (-c_s \tau) - b_y (c_s \tau)) \right) + \left( \frac{\alpha \beta \alpha \beta \nu \sigma}{2c^2} (b_z (-c_s \tau) - b_z (c_s \tau)) \right) + \\
\left( \frac{\alpha \beta \alpha \beta \nu \sigma}{2c^2} (p (-c_s \tau) - p (c_s \tau)) \right)$
for $y$ - lateral component of velocity (for another direction $z$ lateral directions change their places):

$$V_y = \frac{\alpha_f^2 c^2 \beta_y^2 (v_y (c_s \tau) + v_y (-c_s \tau))}{2c^2} + \frac{\alpha_s^2 c^2 \beta_y^2 (v_y (c_f \tau) + v_y (-c_f \tau))}{2c^2} + \frac{\alpha_s^2 c^2 \beta_y \beta_z (v_z (c_f \tau) + v_z (-c_f \tau))}{2c^2} + \frac{\text{sign} (B_z) \alpha_f c_f \beta_y \alpha_s c_s (v_y (c_s \tau) + v_y (-c_s \tau) - v_x (c_f \tau) - v_x (-c_f \tau))}{2c^2} + \frac{\text{sign} (B_z) \alpha_f^2 c_f \beta_y \beta_z (b_y (c_f \tau) - b_y (-c_f \tau))}{2c^2}$$

for $y$ - lateral component of the magnetic field (for another direction $z$ lateral directions changes their places):

$$B_y = \frac{\alpha_f^2 \beta_y^2 (b_y (c_s \tau) + b_y (-c_s \tau))}{2} + \frac{\alpha_s^2 \beta_y^2 (b_y (c_f \tau) + b_y (-c_f \tau))}{2} + \frac{\beta_y^2 (b_y (c_a \tau) + b_y (-c_a \tau))}{2} + \frac{\text{sign} (B_z) \alpha_f c_f \beta_y \beta_z (b_z (c_f \tau) + b_z (-c_f \tau) - b_x (c_f \tau) - b_x (-c_f \tau))}{2} + \frac{\alpha_s^2 \beta_y \beta_z (b_z (c_a \tau) + b_z (-c_a \tau))}{2}$$

for the pressure:

$$P = \frac{\rho \alpha_f^2 c_f (v_x (-c_f \tau) - v_x (c_f \tau))}{2} + \frac{\sqrt{\alpha_f \alpha_s \beta_y c (b_y (c_f \tau) + b_y (-c_f \tau) - b_y (c_s \tau) - b_y (-c_s \tau))}}{2c}$$
The final equation for the electricity field:

\[ E_{x,i,k+1/2,l+1/2} = \frac{1}{4} (B_{y,i,k+1/2} U_{x,i,k+1/2} - B_{z,i,k+1/2} U_{y,i,k+1/2} + B_{y,i,k+1/2} U_{z,i,k+1/2} - B_{z,i,k+1/2} U_{y,i,k+1/2} + B_{y,i,k+1/2} U_{x,i,k+1/2} - B_{z,i,k+1/2} U_{y,i,k+1/2}) \]

\[ E_{y,i+1/2,k,l+1/2} = \frac{1}{4} (B_{z,i+1/2,k,l} U_{y,i+1/2,k,l} - B_{x,i+1/2,k,l} U_{y,i+1/2,k,l} + B_{x,i+1/2,k,l} U_{z,i+1/2,k,l} - B_{z,i+1/2,k,l} U_{y,i+1/2,k,l} + B_{x,i+1/2,k,l} U_{y,i+1/2,k,l} - B_{z,i+1/2,k,l} U_{y,i+1/2,k,l}) \]

\[ E_{z,i+1/2,k+1/2,l} = \frac{1}{4} (B_{x,i+1/2,k,l} U_{y,i+1/2,k,l} - B_{y,i+1/2,k,l} U_{x,i+1/2,k,l} + B_{y,i+1/2,k,l} U_{x,i+1/2,k,l} - B_{x,i+1/2,k,l} U_{y,i+1/2,k,l} + B_{x,i+1/2,k,l} U_{y,i+1/2,k,l} - B_{y,i+1/2,k,l} U_{x,i+1/2,k,l}) \]

APPENDIX

Speed of reactions, and also associated with them functions of cooling/heating has a following form. Speed of reactions Molecular hydrogen formation \((cm^3s^{-1})\) and further:

\[ k_1 = \frac{3 \times 10^{-17} \sqrt{T/100} \times n/n_H}{1 + 0.4 \sqrt{T/100} + 0.2(T/100) + 0.08(T/100)^2} \]

heating function in \((ergs \times cm^{-3}s^{-1})\) and further:

\[ \Gamma_1 = 7.2 \times 10^{-12} \frac{n_{H_2}/n}{1 + 4/0.416 \times 0.327 x} \]

where \(x = log(T/10^4)\).

Speed of reaction for molecular hydrogen first dissociation:

\[ k_2 = \begin{cases} 6.11 \times 10^{-14} \exp (-2.93 \times 10^4/T) & T > 7390 \\ 2.67 \times 10^{-15} \exp (-6750/T)^2 & T \leq 7390 \end{cases} \]

cooling function:

\[ A_2 = n_{H_2} \frac{L_H}{1 + L_H/L_L} \]

where

\[ L_H = \begin{cases} 3.9 \times 10^{-19} \exp (-6118/T) & T > 1087 \\ 10^{-19.24+0.474x-1.247x^2} & T \leq 1087 \end{cases} \]

\[ L_L = \left(n_{H_2}^{0.77} + 1.2 n_{H_2}^{0.77}\right) \times \begin{cases} 1.38 \times 10^{-22} \exp (-9243/T) & T > 4031 \\ 10^{-22.9-0.553x-1.148x^2} & T \leq 4031 \end{cases} \]
where \( x = \log(T/10^4) \).

Speed of reaction for molecular hydrogen second dissociation:

\[
k_3 = \begin{cases} 
5.22 \times 10^{-14} \exp \left( -3.2210^4/T \right) & T > 7291 \\
3.17 \times 10^{-15} \exp \left( -(4060/T) - (7500/T)^2 \right) & T \leq 7291
\end{cases}
\]

cooling function

\[
A_3 = n_{H_2} \frac{L_H}{1 + L_H/L_L}
\]

where

\[
L_H = 1.1 \times 10^{-13} \exp \left( -6744/T \right)
\]

\[
L_L = 8.18 \times 10^{-13} \left( n_H k_H + n_{H_2} k_{H_2} \right)
\]

where

\[
k_{H_2} = 6.29 \times 10^{-15} \times 1.38 \times f(T)/f(4500)
\]

where \( f(T) = \sqrt{T} \alpha \exp \alpha, \alpha = 1 + (kT)^{-1}, k \) – Boltzmann constant.

Speed of reaction for molecular hydrogen photodissociation:

\[
k_4 = \xi_{\text{diss}}(0) f_{\text{shield}}(N_{H_2}) f_{\text{dust}}(A_V)
\]

where \( \xi_{\text{diss}}(0) = 3.3 \times 1.7 \times 10^{-11} \) – unshileded photodissociation rate (Draine 1978), \( f_{\text{dust}}(A_V) = \exp(-\tau_{d,1000}(A_V)) \) – absorption rate on dust (Draine & Bertoldi 1996), where \( \tau_{d,1000}(A_V) = 3.74A_V = 10^{-21}(N_H + N_{H_2}) \) – optical depth on dust particles on wavelength \( \lambda = A_{1000} \), where \( N_H \) and \( N_{H_2} \) – column density. The function of the coefficient of self-shielding can be approximated (Draine & Bertoldi 1996):

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

where \( x = N_{H_2}/5 \times 10^{10} \) m², \( b_5 = b/10^7 \) m/s, where \( b \) – the parameter of Doppler expansion, heating function

\[
\Gamma_4 = 6.4 \times 10^{-13} \times k_4 n_{H_2}
\]

Speed of reaction for Cosmic Ray ionization \( k_5 = 6 \times 10^{-18} n_{H_2} \), heating function \( \Gamma_5 = 1.92 \times 10^{-28} n \).

Speed of reaction for collision ionization:

\[
k_6 = \exp \left( -32.7 + 13.5 \log(T) - 5.7 \log^2(T) + 1.5 \log^3(T) - 0.3 \log^4(T) \right)
\]

\[
+3.4(-2) \log^5(T) - 2.6(-3) \log^6(T) + 1.1(-4) \log^7(T) - 2.1(-6) \log^8(T) \]

cooling function

\[
A_6 = 2.18 \times 10^{-11} k_6
\]

Speed of reaction for Radiative recombination:

\[
k_7 = 10^{-10.75+4.4 \times 10^{-4} (-0.87)^2+0.08+3(-3) \times 4} 
\]

where function \( x = \log(T) \) and cooling function

\[
A_7 = 4.65 \times 10^{-30} \times T^0.94 \times \left( \frac{\exp(-0.75 \times 10^{-20}(N_H + N_{H_2})/n_e)}{n_e} \right)^{0.74/T^{0.668}}
\]

Speed of reaction for EI recombination on grains:

\[
k_8 = \frac{12.25 \times 10^{-14}}{1 + 8.074(-6) \times 10^2.756(1 + 5.087(2) \times T^{1.586(-2)}10^{-1.8892-4.4(-5)\log(T)})}
\]

cooling function

\[
A_8 = 5.7 \times 10^{-26} \times (T/10^4)^{0.8}
\]