The numerical modelling of MHD astrophysical flows with chemistry

I Kulikov, I Chernykh and V Protasov

1 Institute of Computational Mathematics and Mathematical Geophysics SB RAS, Novosibirsk, Russia
2 Novosibirsk State Technical University, Novosibirsk, Russia
3 Novosibirsk State University, Novosibirsk, Russia

E-mail: kulikov@ssd.ssc.ru

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 chemodynamics of the hydrogen while the turbulent formation of molecular clouds is modeled.

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 hydrodynamic instabilities and ram-pressure mechanism in galactic clusters [1] was studied; primarily radial orientation of the magnetic field in Virgo cluster outside the central area was defined [2], and comparison of magnetic field with radio observation was carried out [3]. The structure of magnetic field in spiral arms of the M51 galaxy was investigated in [4], and the evolution of the disk galaxy with consideration of the influence of magnetic field was described in [5]. 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 [6, 7]. For the problems of evolution of MHD instabilities, the power spectrum [8], subalfven flows [9], and starburst rate [10] were studied, and the comparison of different codes on the problem of supersonic turbulence was made in [11]. For the problems connected with the stellar wind, the MHD simulation is also necessary. Thus, the turbulence in stellar wind was described in [12], one-dimensional MHD model of interaction of stellar wind with 67P/Churyumov-Gerasimenko comet in [13], Halley comet [14], and also gas planet [15, 16] was built. In addition, the similar problems of interaction between stellar wind and stars [17] are worth noting.

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 a hybrid method developed earlier with the combination of operator splitting approach and Godunov method in its basis [18-29]. 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 [30]. 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:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0
\]

\[
\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \mathbf{v}) = S_i
\]

\[
\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v} - \mathbf{B} \mathbf{B}) = -\nabla p^* - \rho \nabla \Phi
\]

\[
\frac{\partial \rho E}{\partial t} + \nabla \cdot ((\rho \rho^* \mathbf{v} - \mathbf{B} \cdot \mathbf{v})) = - (\rho \mathbf{v} \cdot \nabla \mathbf{v}) + \Gamma - \Lambda
\]

\[
\frac{\partial \rho \varepsilon}{\partial t} + \nabla \cdot (\rho \varepsilon \mathbf{v}) = - (\gamma - 1) \rho \varepsilon \nabla \cdot \mathbf{v} + \Gamma - \Lambda
\]

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

\[
\triangle \Phi = 4\pi G \rho
\]

the condition of divergency free of magnetic field is

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

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

The numerical method for solving the system of gravitational multicomponent magnetic hydrodynamics is based on a combination of operator splitting approach and Godunov method with using of the piecewise-parabolic method on a local stencil. This method consists of the following stages:

(i) eulerian stage, where 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;

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

(iii) lagrangian stage, where the advection of density, momentum, full, and internal energy happens;

(iv) solving of homogeneous differential equations in each cell of computational domain to determine the concentration of the gas mixture;

(v) consideration of subcell cooling/heating processes;
(vi) regularization of numerical solution;
(vii) solving the Poisson equation to evaluate the 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. Chemistry

Chemical reactions for the $i$-th component of the mixture are considered in the following form:

$$\frac{dn_i}{dt} = C_i(T, n_j) - D_i(T, n_j) n_i$$

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:

$$n_i^{t+\tau} = n_i^t + \tau \frac{C_i - D_i n_i^t}{1 + \tau D_i}$$

We understand that it is, possibly, not the best way and, for example, using the code KROME [31] is more efficient but a similar approach was successfully used in works [32, 33].

2.2. Subgrid physics

To consider the subgrid physics the following equations are solved:

$$\frac{\partial \rho E}{\partial t} = \Gamma - \Lambda$$
$$\frac{\partial \rho \varepsilon}{\partial t} = \Gamma - \Lambda$$

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.

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 $[256pc]^3$ with vertical component of magnetic field, uniform initial concentration of atoms $n = 5 \, \text{cm}^{-3}$, initial random perturbation with speed $v_{\text{rms}} = 10 \, \text{km/s}$, initial value of plasma parameter $\beta_{th} = 8\pi \rho_0/B_0^2 = 25$, initial value of turbulent plasma parameter $\beta_{turb} = 8\pi \rho v_{\text{rms}}^2/B_0^2 = 25$, alfvénic Mach number $M = 3.52$, was considered. The following eight reactions from [32], was examined:

(i) Molecular hydrogen formation [34];
(ii) Molecular hydrogen first dissociation [35];
(iii) Molecular hydrogen second dissociation [36];
(iv) Molecular hydrogen photodissociation [32];
(v) Cosmic Ray ionization [32];
(vi) Collision ionization [37];
(vii) Radiative recombination [38];
(viii) EI recombination on grains [39].

Effective adiabatic index was used in the following form:

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

where \(n_H\) is the concentration (in cm\(^{-3}\)) of hydrogen, \(n_e\) is the concentration of electrons, \(n_{H_2}\) is the concentration of molecular hydrogen. Behaviour of concentration of different forms of hydrogen, which mostly was ionized, and molecular hydrogen was a several thousandth of a percent (see fig. 1), was modeled with using of code ChemPAK [40] 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.

![Figure 1. Behaviour of concentrations with temperature of region \(T = 1000\) K and \(T = 5000\) K. Rapid process of ionization within the time period \(10^{11} < t < 10^{11.5}\) s for both temperatures is taking a place.](image)

The results of the simulation are shown in figure 2. The formation of some small waves of density in the moments \(t = 10\) and \(t = 14\) Myr are 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 Alfven speed on the gas density (see fig. 3a), and dependence of cosine of an angle of collinearity between velocity and vector of magnetic field on the gas density (see fig. 3b). It is clear from the figures, that for Alfven Mach number the correlation \(\mathcal{M} \sim n^2\) is traced (it is shown with white line), and the most part of the cloud \(n > 10cm^{-3}\) is in the over-Alfven region (see fig. 3a). The reason of emergence of such mode is in the magnetic turbulent interstellar medium in trans Alfven mode \(\mathcal{M} \sim 1\) with \(n \sim 1\). With such densities (see fig. 3b) 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 Alfven with Mach number \(\mathcal{M} > 100\).
Figure 2. Problem of chemodynamics of evolution of MHD turbulence of interstellar medium. Concentration of the gas in cm$^{-3}$ in moments of time $t = 10$ Myr (left), $t = 14$ Myr (middle), $t = 15$ Myr (right) are given in figure. After the process of hydrogen ionization, the cloud structures are formed in the numerical experiment (512$^3$ grid size was used).

Figure 3. The problem of chemodynamics of evolution of MHD turbulence of the interstellar medium. Dependence of Alfvén speed on gas density (a), and dependence of cosine of an angle of collinearity between velocity and vector of magnetic field on gas density (b) are shown in figures.

4. 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. Chemodynamics of hydrogen during the process of turbulent formation of molecular clouds were modeled.

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