Numerical modelling of the neutral hydrogen dynamics for astrophysical problems

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Abstract. Chemistry plays an important role in many astrophysical processes such as gravitational collapse, the evolution of disks, stars formation. The most of chemical processes for astrophysical problems are presented in classical notation for reactions. In order to simplify the usage of different kinetic schemes in large numerical simulation for solving astrophysical problems, we present the modification of CHEMPAK chemistry package developed by authors early. This modification consisting of the database for storing and editing kinetic, schemes, visual chemistry editor, pre-processor for translation target kinetic scheme to the system of ordinary differential equations (ODE) and a lot of open source ODE solvers such as RADAU5, DLSODES. The pre-processor can translate target kinetic scheme to the ODE system in Fortran or C++ notation for easy usage with a wide selection of mesh or mesh-less hydrodynamic codes. We present the kinetics study of molecular hydrogen formation process, and coupling the AstroPhi mesh hydrodynamic code, as an example of the new CHEMPAK modification usage.

1. Introduction

Last decades the astrochemistry problems became very popular due to a large amount of observational data. Over 150 chemical species were detected in the interstellar medium with more than 50 chemical compounds consisting of five or more chemical elements [1]. The most of astrophysical problems such as the supernova explosion [2] or other includes chemical or nuclear reactions as the very important part of the research. For example, the problems of the dynamics of molecular clouds and their chemical evolution [3, 4], and the chemical evolution of dwarf galaxies [5, 6, 7] can be formulated in one context. The chemical evolution of disk galaxies was modeled according to the different mass distribution [8] for the next problems: the evolution of the Milky Way [9, 10], the study of the metallicity of disk galaxies [11], the evolution of galaxies with galactic wind [12], the galactic halo [13]. Of particular interest are the chemical evolution of molecular clouds and the formation of complex elements up to water and alcohols in masers [14, 15, 16, 17]. It is very important that the complex molecules, which was observed in the interstellar medium, can be formed in ice mantles on interstellar grains. Numerical simulation for this kind of problems plays an important role because experimental researches are very difficult and expensive due to the strong physical conditions of experiments.

Currently, there are practically no astrochemistry codes that can be used as a part of the existing hydrodynamic codes, since in fact, they represent additional procedures describing a separate reaction in the form of a numerical ODE solution [18] or several reactions in the form
of the explicit formula [19, 20]. At this moment, the best-known KROME code is using as the chemistry package for a wide range of astrophysical simulations [21]. In our future work, we are planning to create an alternative code primarily by using HPC (high-performance computing) optimized [22] ordinary differential equations (ODE) solvers for stiff ODE systems.

2. CHEMPAK chemistry package

Figure (1) shows architecture of ChemPAK chemistry code. ChemPAK consists of network database, computational modules and visual interface. User can create and edit systems of chemical equations with unlimited number of equations with easy-to-use interface, translate systems of chemical equations to systems of ODE, add some new equations to the translated system and solve this system by using one of ChemPAK computational modules. ChemPAK can work with the systems of chemical reactions stored in the network database or obtained via the package interface. Then the program automatically generates a numerical model of the chemical reaction system and makes the computations. Thus, a user of ChemPAK can obtain the results of numerical modeling of direct chemical kinetics problem, adjust the chemical kinetic scheme, and promptly evaluate the resulting scheme. ChemPAK chemistry code [23, 24] was created for numerical simulation of direct chemical kinetics problems and preparation of data for using it in different CFD solvers. There are a lot of solvers included in code such as RADAU5, ROCK4, author’s solver which is based on a BDF (Backward Differentiation Formula) method. Figure (2) shows the result of numerical simulation of molecular hydrogen dynamics for astrophysical problem [19, 20].

3. The hydrodynamical model

To account for chemical reactions, we will consider the equations of multicomponent single-speed component gravitational hydrodynamics equations, which is written in Euler coordinates:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0,$$

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \vec{u}) = -s_i,$$
Figure 2. The evolution of molecular hydrogen for multi-species chemistry processes in astrophysics.

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

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

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

\[
\rho E = \frac{1}{2} \rho \vec{u}^2 + \rho \varepsilon,
\]

\[
p = (\gamma - 1) \rho \varepsilon = S \rho^\gamma.
\]

The Poisson equation can be written as:

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

where \(p\) – gas pressure, \(\rho_i\) – density of i-th species, \(s_i\) – speed of formation of i-th species, \(\rho\) – density of gas mixture, \(\vec{u}\) – speed gas component, \(\rho E\) – density of total mechanical gas energy, \(\Phi\) – gravitational potential, \(\varepsilon\) – density of internal energy of gas, \(S\) – entropy, \(\gamma\) – adiabatic index, \(\Lambda\) – function of Compton cooling, \(\Gamma\) – function of heating from chemistry.

4. The chemistry of neutral hydrogen

Hydrogen molecules in intergalactic space are formed on a surface of particles and dissociated space radiation. Assuming that the density of gas is proportional to the density of particle concentration of molecular hydrogen [25] because of the good mixing of particles and gas in our model, it can be written 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 \( n_H \) – concentration of molecular and atomic hydrogen, \( N_{H_2} \) – the column density of molecular hydrogen, speed of formation of molecular hydrogen on dust is set by function \( R_{gr}(T) = 2.2 \times 10^{-18} \sqrt{T} \text{ s}^{-1} \), where \( S = 0.3 \) – efficiency of formation of molecular hydrogen on dust \[27\], speed of ionization of hydrogen by the space beams is set by function \[28, 29\] \( \xi_H = 6 \times 10^{-18} \text{ s}^{-1} \), where \( A_e \) – extinction \[30\]. Photodissociation rate in the form of \[31\] \( \xi_{\text{diss}}(N_{H_2}, A_V) = \xi_{\text{diss}}(0) f_{\text{shield}}(N_{H_2}) f_{\text{dust}}(A_V) \), where \( \xi_{\text{diss}}(0) = 3.3 \times 1.7 \times 10^{-11} \text{ s}^{-1} \) – unshielded photodissociation rate \[32\], \( f_{\text{dust}}(A_V) = \exp(-\tau_{d,1000}(A_V)) \) – absorption rate on dust \[31\], where \( \tau_{d,1000}(A_V) = 3.74 A_V = 10^{-21} (N_H + N_{H_2}) \) – optical depth on dust particles on wavelength \( \lambda = \lambda_{1000} \), where \( N_H \) and \( N_{H_2} \) – column density. The function of the coefficient of self-shielding can be approximated \[31\]:

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

where \( x = N_{H_2}/5 \times 10^{10} \text{ m}^2 \), \( b_5 = b/10^7 \text{ m/s} \), where \( b \) – the parameter of Doppler expansion.

After calculation of molecular hydrogen concentration \( n_{H_2} \), the adiabatic index \[3\] is defined:

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

The equation for the description of hydrogen concentration dynamics has the analytical solution which was used in realization.

5. The Sedov-like problem with noncentral explosion

For a model Sedov-like problem with noncentral explosion, let us consider a hydrostatically equilibrium density profile:

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

and pressure profile:

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

In cloud on x-axis injected pressure for \( x = 0.25 \) is equal to \( P = 1000 \) and normal distribution for the velocity vector. The results of the simulation \[33\] are shown in the figure (3). Noncentral explosions of stars are of interest first of all in the context of the research of SNIa. It can be seen from figure (3) that even in the case of a noncentral explosion, a spherically symmetric shock wave is formed with a maximum temperature on it, where reactions involving hydrogen take place actively. In the following, we will describe in more detail the mechanism of detonation SNIa based on the merger of two CO dwarfs and on base C+C reactions.

6. Conclusion

In order to simplify the usage of different kinetic schemes in large numerical simulation for solving astrophysical problems, we present the modification of CHEMPAK chemistry package developed by authors early. This modification consisting of the database for storing and editing kinetic, schemes, visual chemistry editor, pre-processor for translation target kinetic scheme to the system of ordinary differential equations (ODE) and a lot of open source ODE solvers such as RADAU5, DLSODES. The pre-processor can translate target kinetic scheme to the ODE system in Fortran or C++ notation for easy usage with a wide selection of mesh or mesh-less hydrodynamic codes.
Figure 3. The nondimensional density in time 0 (a), 0.01 (b), 0.02 (c), 0.03 (d), 0.04 (e), 0.05 (f) after noncentral explosion.

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