Generating Automatic Network Reduction Module for Chemical Hydrodynamics Simulations

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Abstract. Since molecules exist in the interstellar cloud and they affect the hydrodynamic evolution through their formation and destruction, physical states of the actual interstellar cloud are different from calculations of conventional hydrodynamics simulations. Furthermore, in the case of running star-forming simulations, conventional hydrodynamics models are not enough to explain molecular lines emitted from clouds such as those detected from the ALMA observatory. In order to simulate the chemical evolution of a hydrodynamic cloud, building an efficient chemical network that contains relevant chemical reactions is crucial for cutting down the computation cost. A key factor for generating an efficient chemical network is to avoid using an abnormally small network that contains only a few reactions because using too small a network does not simulate the effects of molecules accurately. There already exist a few chemical hydrodynamics simulation codes, which provide pre-built reduced networks. Although those pre-built networks make the simulations simple and light, they cannot be used universally for various clouds under diverse initial chemical compositions and environmental conditions. Therefore, it is necessary to build a more flexible network according to the conditions of the model. In this study, we propose to make an automatic network reduction module which builds an optimized closed network corresponding to the specific simulation conditions. As a preliminary result, we test our module with simple primordial test clouds by comparing our results with those obtained with the full network. In the future study, we will validate our reduction module for primordial cloud models and expand its usage to various physicochemical cases such as AGB stars.

1. Introduction
Hydrodynamics (HD) simulations play a crucial role in studying numerous celestial phenomena because many astronomical objects can be treated as fluid. However, there are some situations where HD simulations are not sufficient alone. For example, magnetohydrodynamics (MHD) is often required in order to explain astronomical phenomena that occur in the plasma states of the material [1]. Another recent example is chemical-hydrodynamics (CHD) simulations which trace the change of chemical species as a function of time while running HD simulations. The need for CHD simulations emerged in recent years due to the ALMA observations of tremendous

1 CHD is generally known as physicochemical hydrodynamics (PCHD) as well.
molecular lines, but the CHD simulations have not been actively performed compared to HD and/or MHD simulations.

A crucial reason for lacking the CHD simulations is the limitation of computational resources. In order to trace the change of all the relevant chemical species, the abundance of each molecule (or atom) must be treated as a variable in the code. Because tracing a decent number of species is usually required in the CHD simulations in order to explain the observed molecular lines, the realistic CHD simulations need to take at least a few tens of variables. For the conventional three dimensional (3D) HD simulations, it is sufficient to use six or seven variables (density, three components of velocity, internal energy, pressure and/or temperature depending of equation of state). Therefore, the 3D CHD simulations require more computational resource than the 3D HD simulations by at least a factor of three. Furthermore, the more species are included, the more reactions need to be solved. This also increases the computing time. As a result, CHD simulations are generally more challenging than HD and MHD ones.

It is possible, however, to perform these challenging simulations efficiently by using a selected network (a network is composed of species and reactions) which is optimized for the problem-specific situations. The optimization can be done by reducing the number of chemical species and reactions from the large original network which includes all the known species and reactions. This approach has been tried already and there are some CHD simulators which use a pre-built reduced network [2]. Most CHD simulators which use pre-built networks select the species and reactions manually and pre-built networks made in this way may not guarantee accurate simulations under diverse physical and/or chemical conditions. Meanwhile, Wiebe et al. [3] suggested a sturdy method to make an automatic reduction. They calculated priorities of each species and/or reaction to determine which species and reactions are reducible. Although their method is well-organized, it shows significant errors during CHD simulations, especially for the case of the diffuse gas cloud. Therefore, it is still necessary to build a proper automatic module that makes an optimized closed network for a given physicochemical condition by reducing the large original network. In this study, we propose to develop such an automatic module and present our preliminary algorithm and results obtained with simple tests.

In the following section, we explain how the reduction module works and the algorithm of the module. We also test our reduction module. We choose two simple test models (Section 3). We evolve them with both the reduced network built by our reduction module and the full (i.e., original) network and compare two results (Section 4). We summarize our study and discuss the future work in the final section.

2. Reduction Module

2.1. Role of Reduction Module

A grid-based hydrodynamics simulator is designed to update the physical states of gas (or any fluid) over time at the segmented cells which are combined together to cover the entire computational domain. As mentioned earlier, on top of the hydrodynamics part, the CHD simulator additionally updates the abundances of chemical species by calculating the rate equations that contain the chemical reactions among the chemical species. Therefore, the CHD simulator requires the input information on the chemical composition of the model cloud and the list of chemical reactions related to the chemical composition. Because the abundances of the chemical species are also affected by environmental conditions such as cosmic rays, background ultraviolet (UV) radiation, and visual extinction, it is also necessary to implement these environmental parameters into the CHD simulator.

Figure 1 shows schematically how the CHD simulator works. Both the initial composition and the physical parameters determining the environmental conditions, which are specified by the problem, are the input not only to the simulator itself but also to the network reducer (i.e., our automatic reduction module). The network reducer reduces both species and reactions from
the full (original) network and builds a reduced network which is used now as input to the CHD simulator. Without the reduction process, the full network is used as the input to the simulator, but in this case the simulator does unnecessary calculations for the species and reactions that are not relevant to the problem. Because these dummy calculations are just a waste of the computing resources, the reduction module can increase the computing efficiency.

Since the currently available full network includes more than 400 chemical species and 6000 reactions, it is not a trivial task to build an efficient automatic reduction module which works for all the various cases. In the following subsection, we introduce the algorithm that we use for the reduction. Note that the current version of our algorithm is still under development. In the final section, we will briefly mention what will be required to improve the current algorithm.

2.2. Algorithm of Reduction Module
The flowchart of our reduction algorithm is shown in Figure 2. Before explaining the details, it is worth mentioning an important rule for the reduction process. A network both full and reduced must be closed. That is, all the species in the network must interact with the others through the reactions in the network. Without violating this, our algorithm reduces the full network according to the following steps.

First, by using the information on the composition of the problem, our module identifies zero-abundance reactants which do not appear at all during the period of simulations and removes the species of zero-abundance reactants and the reactions which involve the zero-abundance reactants.

The second step eliminates reactions from the full network according to the physical conditions. In this step, the reduction module determines whether the model cloud has the proper conditions such as temperature and environments for certain reactions to occur. For example, when the cloud has neither background radiation nor cosmic ray, most of photodissociation reactions are removed.

In the final step, we tried to reduce the network further by checking out individual reaction rates. When the rates of certain reactions are very small (i.e., smaller than the threshold value of $10^{-20}$), our reduction module ignores them. But care needs to be taken in order not to violate the rule that the reduced network must be closed. When used in the chemical evolution, the reduction module with this step may produce different amounts of some chemical species in

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{The schematic figure showing how the CHD simulator works. Our network reduction module is indicated by a yellow box.}
\end{figure}
comparison with those calculated with the full network. However, as long as the difference is not significant, the reduced network can be used in the place of the full network reducing the computing resources and time in the chemical evolution calculations.

![Figure 2. The schematic algorithm of the reduction module](image)

### 3. Test Models

We tested our reduction module for a simple static situation. In this case, the dynamical motion of the fluid can be ignored and the abundance change of chemical species can be traced by solving the rate equations only. In other words, it is sufficient to use a chemical evolution code as the simulator in Figure 1 without calculating any hydrodynamics update. We used Astrochem (version 0.7) for the calculation of the chemical evolution [4]. Astrochem numerically solves the rate equations which are in fact ordinary differential equations. When we consider all of formation and destruction reactions for an arbitrary molecule AB, the ordinary differential equation for the abundance evolution of this molecule is

\[
\frac{d}{dt} N(AB) = \sum_i k_i \prod_a N(X_a) - N(AB) \sum_j k_j \prod_b N(Y_b),
\]

where \(X_a\) is an \(a\)-th reactant of the \(i\)-th formation reaction and \(Y_b\) is a \(b\)-th reactant of the \(j\)-th destruction reaction of molecule AB. A set of coupled equations for participating species are solved together by Astrochem.

Astrochem can also handle the effects of various physicochemical environments such as cosmic ray and photon by considering reactants or products in the above equation as cosmic ray or photon. Astrochem uses the full network based on the Ohio State University (OSU)
astrochemistry database (version osu_01_2009) which contains 6046 reactions and 468 species. Note that we also used the OSU database as the full network from which our reduction module builds the reduced network.

We considered two simple model clouds for the test of the static situation. The first cloud contains only hydrogen molecule and the second cloud is the simplest two-element cloud which contains helium and molecular hydrogen. In both cases, all hydrogen atoms are bounded as diatomic molecular state at the initial time. So, we set the abundance of $H_2$ as 0.5 in both test models (Table 1) because the abundances of $H$, $H_2$, $H^+_3$ have a relation, $N(H) + 2 \times N(H_2) + 3 \times N(H^+_3) = n(H)$, where $N(X)$ and $n(H)$ indicate the number density of a given species $X$ and hydrogen nuclei, respectively, in unit of cm$^{-3}$ [4]. We set the abundance of helium for the second model cloud as 0.14 which is selected from [6].

| Species | Abundance ($/n(H)$) |
|---------|---------------------|
| $H_2$   | 0.5                 |
| He      | 0.14                |

Table 1. Initial abundances in our test models

For our test, we also include the physical and environmental effects. Table 2 shows the physical parameters and their values used in our test. These values are the input parameters to Astrochem.

| Density | CRIR | UV intensity | Temperature | Visual Extinction |
|---------|------|--------------|-------------|------------------|
| $n(H) = 500$ cm$^{-3}$ | $1.3 \times 10^{-17}$ | 1.0 Draine$^2$ | 100 K | 5.0 magnitude |

$^2$ See [7] for a description of Draine units.

Table 2. Physical and environmental parameters in our test models

4. Results

By using the initial composition and the physical conditions of our two test models as the input information, our reduction module builds the reduced networks that correspond to each model, respectively. We calculate the chemical evolution of two test models with the reduced network and compare the results with those evolved with the full network. Table 3 shows the size of the reduced network and the computational gain for two simulations. The list of species in each reduced network is posted at Tables 4 and 5. When we used the reduced network for the two tests, the computing time got decreased as small as 1/80th of that run with the full network.

| Model   | Size of reduced network$^2$ | Gain |
|---------|-----------------------------|------|
| H-only  | 7 (24)                      | $\sim$ 80  |
| He+H    | 9 (30)                      | $\sim$ 80  |

$^2$ number of species (number of reactions)

Table 3. Size of reduced network and computational gain for our test models

$^2$ See http://faculty.virginia.edu/ericherb/research.html and [5].
4.1. Test Model 1: Hydrogen-only Cloud

Table 4 lists the species in the reduced chemical network for the first test model, the hydrogen-only cloud. The reduced network contains 24 reactions only among these seven species that make it a closed network.

The upper-left and upper-right panel in Figure 3 show the evolution of the seven species obtained with the reduced network and the full network, respectively. At a glance, there seems no significant difference between them, but the fractional difference defined as \[\frac{N(X)_{\text{red}} - N(X)_{\text{full}}}{N(X)_{\text{full}}}\] where \(N(X)_{\text{red}}\) and \(N(X)_{\text{full}}\) are the abundance of species \(X\) calculated with the reduced and full network, respectively, looks apparent for two species, tri-hydrogen cation (\(\text{H}_3^+\)) and electron (\(e^-\)) although the maximum errors for these two species are 4.3% (\(\text{H}_3^+\)) and 0.2% (\(e^-\)) throughout the entire evolution of \(10^9\) years (see lower panel in Figure 3). Note that the amounts of produced species from the initial hydrogen molecule are still very small compared to that of hydrogen molecule. Hydrogen atom (\(\text{H}\)) was produced most abundantly, but its amount is still less than 1% of \(\text{H}_2\).

We find that these errors are not based on the third step in the algorithm of the reduction module which removes the reactions with small rates in the full network because the relevant reactions in the reduced network are identical to those in the full network, i.e., the third step did not operate in this case. We speculate that the fractional errors in two species might be caused by the numerical precision of the machine because the maximum values of absolute difference are approximately \(10^{-18}\) for \(\text{H}_3^+\) and \(10^{-9}\) for \(e^-\). We are now investigating the exact cause for these errors, but the overall results show that our reduction module builds the properly reduced network.

| \(\text{H}\) | \(\text{H}^+\) | \(\text{H}^-\) | \(\text{H}_2\) |
|---|---|---|---|
| \(\text{H}_2^+\) | \(\text{H}_3^+\) | \(e^-\) |

Table 4. Chemical species obtained with our reduction module for the first test model, hydrogen-only cloud

4.2. Test Model 2: Helium-containing Hydrogen Cloud

Table 5 shows the species in the reduced network for the second test model, the helium-containing hydrogen cloud. This model cloud containing molecular hydrogen and helium is the simplest two-element model because both elements do not directly react with each other. Although there is a helium hydride cation molecule (hydro-helium, \(\text{HeH}^+\)), its unique production reaction requires the existence of formyl-radical (HCO). Our reduction module recognizes this information and does not import \(\text{HeH}^+\) into our reduced network which contains nine species only because there is no HCO in the initial condition. Again, we check out that our reduced network having nine species and 30 reactions is a closed one.

Figure 4 shows the results for the second test model. As test model 1 does (see Figure 3), the results of this test model show that the chemical evolution of nine species simulated with the full network can be reproduced with the reduced network. However, there is an error in the fractional difference defined as \[\frac{N(X)_{\text{red}} - N(X)_{\text{full}}}{N(X)_{\text{full}}}\] for tri-hydrogen cation (\(\text{H}_3^+\)) (see the bottom panel of Figure 4). As in the test model 1, we find that the third step did not operate either in this case. Thus we also speculate that the fractional errors shown in this test case are caused by the numerical precision of the machine. Note that the evolution pattern of the error looks similar in both test models for tri-hydrogen cation (\(\text{H}_3^+\)) (compare the bottom panel of Figure 3 and 4) and the maximum errors for this cation also have a similar value of 4.3%. The exact reason for this error shown in both test models is under investigation now.
Figure 3. The evolution of seven species for test model 1, the hydrogen-only cloud simulations obtained with the reduced network (upper-left) and the full network (upper-right). Note that the abundance of $H_2$ (thin black lines close to the top boundary) does not change much throughout the evolution and that some curves are overlapped. The lower panel shows the fractional difference defined as $[N(X)_{red} - N(X)_{full}]/N(X)_{full}$ as a function of time.

Table 5. Chemical species obtained with our reduction module for the second test model, helium-containing hydrogen cloud

5. Summary & Future work
In order to reduce the computing resources and time in the CHD simulations, we develop a reduction module which builds a reduced chemical network from the full network. The reduction is done by using the initial composition and the physical conditions of the problem-specific model which are also the initial input to the simulations. We test our reduction module with two simple static clouds by using Astrochem, a chemical evolution code, as a simulator.
Figure 4. The evolution of nine chemical species for test model 2, the helium-containing hydrogen cloud simulated with the reduced network (top-left) and the full network (top-right). As in Figure 3, the abundance of $H_2$ (thin black lines close to the top boundary) does not change much throughout the evolution and some curves are overlapped. The bottom panel shows the fractional difference defined as $[N(X)_{\text{red}} - N(X)_{\text{full}}]/N(X)_{\text{full}}$ as a function of time.

Our two test model clouds contain only hydrogen or both hydrogen and helium, which are relevant for the primordial chemistry simulations. In the future work, we will include more species like deuteron for the more accurate primordial chemistry. We will also test our reduction module which works with more complex chemistry such as a two-element system composed of carbon and oxygen and a three-element system composed of hydrogen, carbon, and oxygen. These models can address the chemical evolution that can occur in the outer part of asymptotic giant branch (AGB) stars as well as in the star-forming region.

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