



Computational Astrochemistry: importance, pitfalls and applications

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Resumen / La astroquímica se encuentra actualmente en su edad de oro gracias a la gran cantidad de datos que proporcionan los telescopios de plato único e interferométricos como APEX y ALMA. Para permitir una mejor comparación e interpretación de los datos de observación, es indispensable hacer un esfuerzo notable también en el aspecto teórico/computacional. Los modelos astroquímicos de última generación son una herramienta poderosa para la interpretación de los datos observacionales y permiten probar las condiciones físicas de las regiones de formación estelar, proporcionando una ventana única para comprender cómo se forman y evolucionan estas regiones. Sin embargo, la inclusión de la microfísica y la química en las simulaciones hidrodinámicas que se basan en la computación requiere información detallada y conocimiento de los procesos químicos básicos. Esto, junto con la amplia gama de escalas espaciales y temporales implicadas en la astrofísica, conduce a un problema computacionalmente costoso. Presentamos aquí las ventajas y los inconvenientes de los modelos astroquímicos y mostramos algunas aplicaciones importantes.

Abstract / Astrochemistry is currently in its golden age thanks to the huge amount of data that single-dish and interferometric telescopes like APEX and ALMA are providing. To allow for a better comparison and interpretation of the observational data it is indispensable to make a noteworthy effort also on the theoretical/computational side. State-of-the-art astrochemical models are a powerful tool for the interpretation of observational signatures and allow to probe the physical conditions of star-forming regions, providing a unique window to understand how these regions are formed and evolved. However, including microphysics and chemistry in computationally intensive hydrodynamical simulations requires detailed information and knowledge of the basic chemical processes. This, together with the wide range of involved spatial and temporal scales in astrophysics, leads to a computationally expensive problem. We introduce here the advantages and pitfalls of astrochemical models, and show some important application.

Keywords / ISM: molecules — hydrodynamics — astrochemistry

1. Introduction

Chemistry is very important for the interpretation of observational data as the entire Universe is permeated by atoms and molecules. The latter are excellent diagnostics of the physical conditions and processes in the regions where they reside, and control the ionization balance, affecting the coupling of magnetic fields to the gas, through important processes like ambipolar diffusion. In addition, molecules are fundamental for the cooling of the gas, which regulates the star formation process.

While observations are very powerful and already provide a lot of information about the observed regions, they only give us a snapshot in time of their evolution. Astrochemical models are then needed to retrieve information on the evolution prior and after the observed stage.

Astrochemistry is a complex multidisciplinary research area, which is now living its golden age in particular thanks to the radio facilities we developed over the last decade. With the advent of ALMA, this discipline has grown exponentially, and has attracted many scientists from different areas, from astrophysicists to

biologists. Since its birth, which goes back to fifties with the development of the first astrochemical models (Kramers & Ter Haar, 1946; Bates & Spitzer, 1951), astrochemistry has changed its objectives and has now become an incredible tool to interpret observational data. This is particularly true for Computational Astrochemistry, i.e. the study of how chemical processes affect the dynamics of galaxies, stars and planets formation via hydrodynamical simulations.

In the following sections, we will present the main pitfalls of computational astrochemistry, and some interesting results.

2. The problem

Chemistry *per se* is a complex problem, which involves many different processes. Beyond the standard gas-phase reactions, indeed, in regions where freeze-out surface chemistry could strongly impact the chemical evolution of the gas.

In the simple case where only gas-phase reactions are considered, we have to face with the solution of a system of coupled ordinary differential equations (ODEs) of the

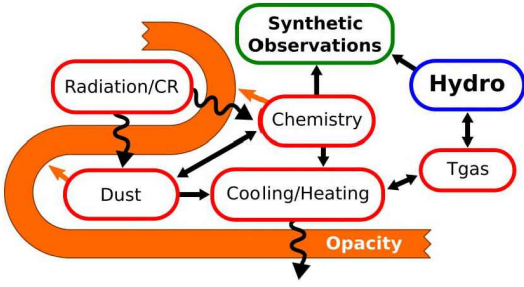


Figure 1: Sketch of chemistry and microphysics complexity.

following form:

$$\frac{dn_i}{dt} = \overbrace{\sum_{lm} k_{lm}(T)n_l(t)n_m(t)}^{\text{formation}} - \overbrace{\sum_j k_{ij}n_i(t)n_j(t)}^{\text{destruction}} \quad (1)$$

where n_i are the chemical abundances number density, k_{lm} and k_{ij} represent the formation and destruction reaction rate coefficients. The above system is extremely CPU demanding, and requires accurate implicit solvers (Bovino et al., 2013). In addition, to build a chemical network is not an easy task, because the uncertainties affecting the rate coefficients are related to the accuracy of the rates itself, and in most of the cases the rates are not available.

Chemistry is also strongly coupled with other physical processes, very interconnected (see Fig. 1), as for instance processes involving radiation, dust-grain physics/chemistry, and in particular the thermal processes, i.e. cooling and heating. When the latter processes are included the system reported in eq. 1 should include the rate change of the temperature in time:

$$\frac{dT}{dt} = \frac{\gamma - 1}{k_B \sum_i n_i} (\Gamma(n, T) - \Lambda(n, T)) \quad (2)$$

with $\Gamma(n, T)$ and $\Lambda(n, T)$ being the cooling and the heating functions in $\text{erg cm}^{-3} \text{s}^{-1}$, γ the adiabatic index, and k_B the Boltzmann's constant. For an overview of different cooling and heating functions see Grassi et al. (2014); Bovino et al. (2016).

As already mentioned in the Introduction, computational astrochemistry is that branch of Astrochemistry which refers to the solution of chemical models necessary to interpret observations. However, models can go from very simple single-zone, which only provide qualitatively results to more complex ones. While the dimension of the problem increases, the chemistry becomes more and more computationally expensive as it should be solved many times, and for many different time-step. Three-dimensional hydrodynamics simulations suffer memory problems because of the huge amount of data that should be stored over the entire time domain. For this reason coupling the chemistry with the hydrodynamics has been, for a very long time, an off limit topic. Furthermore, the chemistry included in hydrodynamical simulations has been kept very simple, with a few species, and some tens of reactions.

With the development of larger and more powerful supercomputing centers it is nowadays possible to include comprehensive chemical networks, and the necessary microphysics to accurately follow the evolution of

the gas in complex simulations (e.g. Glover et al., 2010; Körtgen et al., 2018).

Chemistry couples with hydrodynamics through the energy equation as a source term. Two of the prevailing problems when coupling chemistry and hydrodynamics are i) the adiabatic index (γ), and ii) the mean molecular weight (μ). The first is strongly dependent on the chemical composition of the gas while the second is used to convert pressure \rightarrow energy \rightarrow temperature. In adaptive mesh refinement codes for instance multi-fluid advection and conservation of abundances could provide problems if not handled in the correct way (e.g. loss of chemical flux).

2.1. The package KROME

To alleviate the problem to couple hydrodynamical codes with chemistry, chemical packages have been developed (e.g. Smith et al., 2017). Unfortunately, these codes are still limited to very few and simple species/reactions, and are not prepared to properly describe the chemistry/microphysics in complex environment like galaxies and star-forming regions.

In Grassi et al. (2014), we have presented the package KROME, which is optimised to be included in hydrodynamics codes, and contains a lot of processes. In the last four years, KROME has been employed in several works, exploring a variety of astrophysical problems and conditions. This allows people to avoid a series of typical problems when employing chemistry in simulations, as for instance the environment-dependent assumptions, or the use of numerically unstable solvers.

3. Chemistry in Hydrodynamics: results

Some of the results obtained with KROME, through different hydrodynamical codes are reported in Fig. 2 and Fig. 3, where we show star-forming filaments with deuteration, and a turbulent molecular cloud simulation.

3.1. Star-forming filaments

Deuterium fractionation, i.e. the enrichment of deuterated molecules towards the non deuterated, is considered to be an important chemical tracer of the initial conditions of star-forming regions (Caselli et al., 2003). In highly depleted environments, H_2D^+ is the main ion still available in gas phase. Whether or not H_2D^+ can be used to trace the different evolutionary stages of star-forming regions is not clear. We have recently performed high-resolution three-dimensional MHD simulations of star-forming filaments following deuteration chemistry (Körtgen et al., 2018). We have found that a high-level of deuteration can be reached within one million years, and that dynamical parameters do not strongly affect the results. A typical time-evolution sequence for deuterium enrichment is reported in Fig. 2.

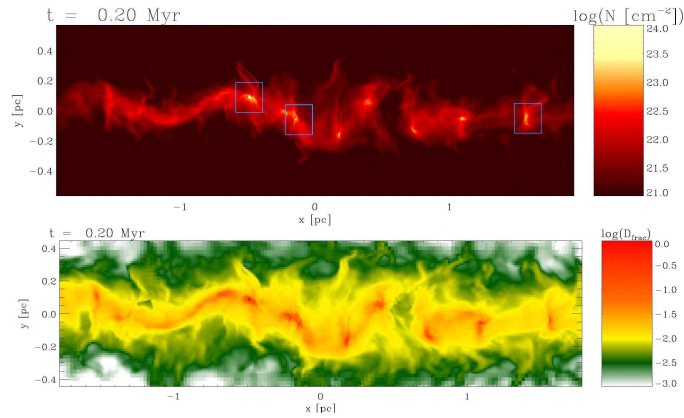


Figure 2: Total column density (top panel) and deuteration (bottom panel). Re-arranged from the collapsing filament simulations of Körtgen et al. (2018). The blue squares represent the most evolved clumps.

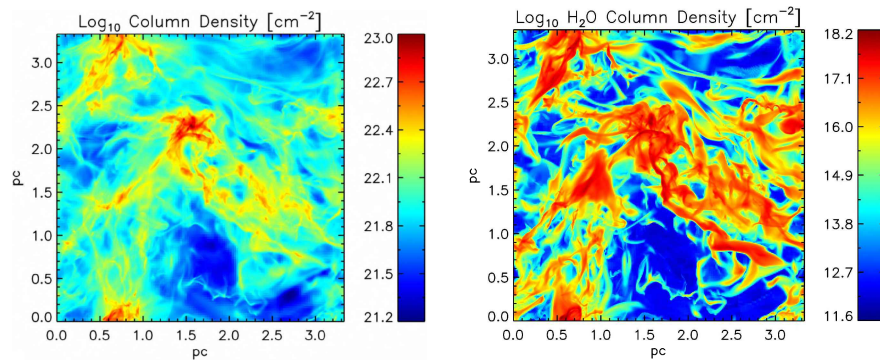


Figure 3: Total column density (left panel) and water column density (right panel), from turbulent molecular cloud simulations. Details of the setup are reported in Grassi et al. (2017); Frostholm et al. (2018).

3.2. Molecular clouds chemistry

In Fig. 3 we report the results of high-resolutions simulations of a molecular cloud patch where we have included a comprehensive H-C-O chemical model. The latter includes 34 species, and 227 reactions and it is an update of the network reported in Glover et al. (2010). We are in particular interested in following CO and H₂O evolution. We employ RAMSES (Teyssier, 2002) to simulate a $(3.3 \text{ pc})^3$ box with an average density of $\rho_0 = 4 \times 10^{-21} \text{ g cm}^{-3}$, with an initial magnetic field of $7 \mu\text{G}$. A constant cosmic ray flux of $1.3 \times 10^{-17} \text{ s}^{-1}$ and a UV interstellar radiation field of 1.69 in units of Habing flux have been used. The initial temperature is set to 20 K. We add six adaptive mesh refinement levels. In Fig. 3 we report the total and the H₂O column density after 5.6 Myr of evolution as plotted from the data of Grassi et al. (2017).

4. Conclusions

We have presented an overview of recent developments of astrochemistry, with particular focus on its computational aspects. The main pitfalls when coupling chemistry with hydrodynamics have been discussed, and the package KROME introduced. Recent results from three-dimensional hydrodynamics simulations have been presented. In particular, results from high-resolution tur-

bulent molecular cloud simulations where we follow a large CO network, and collapsing filaments with deuteration chemistry have been discussed. The results show the importance of including chemistry in hydrodynamics simulations, and the efficiency of doing that via highly optimised packages like KROME.

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