Beauty Out of Darkness: A New Model for Molecular Hydrogen in Galaxy Simulations

Abstract

This research, like much of astrophysics, sits at the intersection of physics, chemistry, and computer science. We begin with a review of the necessary background material.

From its birth shortly after the Big Bang, molecular hydrogen is responsible in shaping the first stars. We explain molecular hydrogen on the quantum mechanical level and the ways in which it interacts with photons and other chemical species. These properties cause difficulty in directly observing molecular hydrogen in space, and we discuss the alternative methods that astronomers use to determine molecular hydrogen content. Molecular hydro- gen is most commonly measured in dense, cold clouds, governed on one side by chemistry and on the other by physics and gravitation. These clouds are the sites of star formation in galaxies, and the correlation between molecular hydrogen and star formation is a current topic of great interest.

Parallel to the observational side of this research is the computational aspect. After showcasing the origins of computational astrophysics, we will introduce the components of modern astrophysical simulations. The first of these components is dark matter, which exerts a gravitational influence on luminous matter without itself interacting with photons. Dark matter simulation techniques are fairly uniform, but astrophysical codes differ in their treatment of gas hydrodynamics, through either smoothed particle hydrodynamics, adaptive mesh refinement, or a moving mesh code. Finally, we will cover the processes unique to astrophysical simulations: stars, supernovae, and black holes.

After this introduction of the relevant research, we will be prepared to discuss the research unique to this work, which is covered in two papers.

In the first paper, we present a model of molecular hydrogen chemistry implemented in the code ramses-rt. ramses-rt is an adaptive mesh grid code where the hydrodynamics are coupled to the radiative transfer of photons. It independently tracks the atomic and ionized species of hydrogen and helium coupled to three photon groups.

Our expansion adds molecular hydrogen chemistry and a fourth photon group involved with its dissociation. We introduce a novel method to handle molecular hydrogen's self- shielding against photodissociation. Several test cases and idealized situations demonstrate our model's robustness compared to analytical solutions and specialized chemistry codes.

Our research culminates in the second paper, where we simulate an isolated, Milky Way-like disc galaxy with full radiative transfer and the molecular hydrogen chemistry. Once vetted on the chemical scale, our model requires no tuning on the galactic scale. We study the molecular hydrogen content of this galaxy through the overall morphology, radial profiles that compare hydrogen species to star formation rate, phase diagrams that reveal the temperature and density state of the gas, to a study of individual molecular clouds and their population statistics.

A compilation of observational data at all these scales compares favourably. The simu- lations allow us to characterize the entire spectrum of molecular gas, especially low-density gas that is difficult to observe. By running this same galaxy at three different resolutions, we also study the effect resolution has on the molecular content of simulated galaxies. We provide a self-consistent picture of the relationship between molecular hydrogen and its galaxy.