Draft version May 14, 2025
Typeset using LaTeX **twocolumn** style in AASTeX631

Proposal of Second-Year Research Project: Probing Cosmic Ray Ionization Rates in Star-Forming Clouds: A Synthetic Observation with STARFORGE Simulations

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ABSTRACT

Cosmic rays are a significant factor influencing various aspects of star formation within molecular clouds, including chemical abundances, gas temperature, and star formation efficiencies. The cosmic ray ionization rate (CRIR) from indirect measurements of star-forming regions are an order of magnitude larger than direct measurements from the Voyager spacecrafts. For this project, I will use numerical simulation data from STARFORGE (Fitz Axen et al. 2024) to examine how cosmic rays affect chemistry of star-forming clouds. I aim to produce synthetic observations of cosmic ray tracers (e.g., H_3^+) to evaluate the accuracy of the CRIRs derived in molecular clouds.

1. INTRODUCTION

Cosmic rays (CRs) are charged particles (electrons, protons, ions) diffusively distributed in the interstellar medium (ISM). They are produced and accelerated primarily by shocks from Galactic supernova remnants (SNRs, e.g., Aharonian et al. 2019; Ackermann et al. 2011). On Galactic scales, CRs are expected to be uniformly distributed due to efficient diffusion. However, the smaller scales relevant to star formation (tens of parsecs), CR density variations become significant and require closer examination (Zweibel 2017; Padovani et al. 2020).

Over the past decade, the influence of low-energy (<1GeV) CRs on star formation has received increasing attention (Padovani et al. 2020). These CRs propagate and interact with atoms, ions, or molecules in the molecular clouds by losing energy. Ionization of atomic and molecular hydrogen (H) is a major channel for energy loss by low-energy CR protons in the ISM. In contrast, higher energy CRs (TeV or above) typically penetrate molecular clouds without significant interaction. CRs also affect cloud dynamics in dense gas by propagating along local magnetic fields, which can be complex in dense regions (Silsbee et al. 2018). The degree of CR ionization determines the coupling between the gas and magnetic fields. Simulations have shown that CR ionization rates decrease with increasing magnetic field strength in collapsing clouds (Padovani et al. 2013, 2014), which may contribute to ambipolar diffusion and facilitate rotational disk formation (Mellon & Li 2009).

Low-energy CRs are primarily responsible for ionizing gas and initiating the formation of various molecular ions. As these CRs also modify the abundances of atomic and molecular species, they play a significant role in shaping the chemical evolution of molecular clouds. Key ions such as H_3^+, OH^+, HCO^+, and HN_2^+ are closely linked to the ionization of molecular hydrogen H_2 (Indriolo & McCall 2012). H_3^+ is particularly important as a CR tracer due to its simple formation pathway and direct production from low-energy CR ionization. A variety of observational evidence suggests that low-energy CRs may be produced locally within star-forming regions (e.g., Ackermann et al. 2011; Yang et al. 2018; Pandey et al. 2024). These CRs are generally attributed to two types of sources: Galactic and local. Galactic CRs are produced by mechanisms such as SNR shocks and stellar winds, forming the so-called Galactic CR spectrum. More recently, local sources have attracted growing attention as they may help explain the high ionization rates observed in protostellar environments (Padovani et al. 2013). These local CRs likely originate from shocks generated by accretion shocks (Padovani et al. 2016) or protostellar jets (Padovani et al. 2021).

CRs in molecular clouds can only be probed indirectly, either through their impact on molecular ion abundances (e.g., H_3^+, OH^+) or through other byproducts

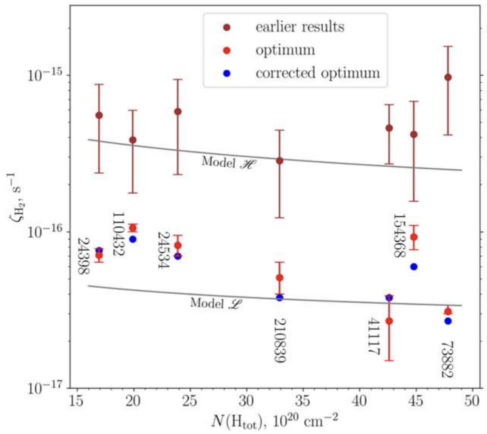

Figure 1. Comparison between H_3^+ measurements from Obolentseva et al. (2024) (corrected optimum) and from previous works such as Indriolo & McCall (2012) (earlier results). Extracted from Figure 7 in Obolentseva et al. (2024).

such as non-thermal synchrotron emission (Padovani & Galli 2018) and gamma-ray radiation resulting from CR interactions with ambient gas (Krumholz et al. 2024). Measurements of the CRIR provides important information about the origin of CRs in molecular clouds and how they propagate. There are two main approaches to measuring the cosmic ray ionization rate (CRIR): direct measurements of CR fluxes and indirect methods based on chemical tracers. The Voyager 1 and 2 spacecrafts have provided direct measurements of CRs beyond the heliosphere, in the local ISM (Cummings et al. 2016; Aharonian et al. 2019). These missions estimated an atomic H (HI) ionization rate of $1.51 - 1.64 \times 10^{-17}\,s^{-1}$. In contrast, indirect estimates typically rely on chemical tracers whose abundances are sensitive to CR ionization. For example, Indriolo & McCall (2012) conducted a survey of H_3^+ absorption in 21 diffuse clouds and inferred an average CRIR for H_2 of $3.5 \times 10^{-16}\,s^{-1}$, an order of magnitude higher than the Voyager measurements. To address this discrepancy, Obolentseva et al. (2024) presented updated H_3^+ measurements using an improved 3-D Galactic extinction map with parsec-scale resolution. Figure 1 compares CRIR values estimated with and without the corrected extinction model. The new analysis systematically reduces the inferred CRIR to $\sim 6 \times 10^{-17}\,s^{-1}$, narrowing the gap with Voyager's direct measurements. However, it remains an open question whether the discrepancies are primarily due to uncertainties in extinction modeling and estimated cloud densities, or whether they also arise from uncertainties in chemical reaction rates and temperature assumptions.

2. STARFORGE STAR FORMATION SIMULATIONS WITH EXPLICIT COSMIC RAY TRANSPORT

In the past two decades, an increasing number of hydrodynamic simulations of galaxy formation and evolution have explicitly incorporated cosmic ray transport (CRT) to investigate the role of CRs in shaping galaxy properties and star formation history (e.g., Jubelgas et al. 2008; Salem et al. 2014; Hopkins et al. 2022). However, most simulations and analytical models of star formation at molecular cloud scales have neglected CR effects, typically assuming a spatially and temporally uniform CRIR on the order of $10^{-17} - 10^{-16}\,s^{-1}$ (e.g., Hopkins 2012; Grudić et al. 2022).

Fitz Axen et al. (2024) presents the hydrodynamics simulations with resolved star formation to explicitly model CRT in molecular clouds, using the STARFORGE framework (Grudić et al. 2021). STARFORGE, built on the Gizmo code (Hopkins 2015), is a comprehensive simulation framework that includes magnetohydrodynamics, self-gravity, stellar dynamics, and various stellar feedback mechanisms including supernovae, protostellar jets, and stellar winds. Fitz Axen et al. explored three key initial parameters: the cloud mass ($M_{\rm cloud}$, fixed at 2,000 $M_\odot$), the CR energy density ($\epsilon_{\rm CR}$, set to either 1 or 10 eV/cm^3), and the CR diffusion coefficient ($D_{||}$, ranging from $\sim 10^{25} - 10^{27}$ cm^2/s). Figure 2 compares the results under different initial conditions. At typical CR energy density (1 eV/cm^3), the difference between simulations with and without CRT is minimal (see upper-left and upper-middle subpanels). However, increasing the CR energy density leads to faster cloud collapse, earlier star formation, and higher star formation efficiency (SFE). On the other hand, low to moderate CR diffusion coefficients ($\sim 10^{25}$ & 10^{26} cm^2 s^{-1}) result in strong CR attenuation within the cloud. In contrast, a sufficiently high diffusion coefficient (e.g. 8.33×10^{26} cm^2 s^{-1}) causes negligible attenuation, making the cloud nearly as transparent to CRs as in the non-CRT model (see upper-middle and lower-middle subpanels). The CRIRs produced in these simulations, ranging from 10^{-19} to 10^{-18} s^{-1}, are systematically lower than observational values, varying with input parameters and physical processes during the evolution (Figure 3), such as CR energy peaks at Time $\sim (1.5-2.2) \times t_{\rm ff}$ induced by stellar winds. Even in high-energy CR models, where the external CRIR is initialized at $\sim 10^{-16}\,s^{-1}$, the resulting CRIR remains lower than the commonly assumed value of $\sim 10^{-17}\,s^{-1}$. Since the CRIR in STARFORGE is directly calculated from the CR energy density within the CRT framework, exploring these differences offers an opportunity to assess

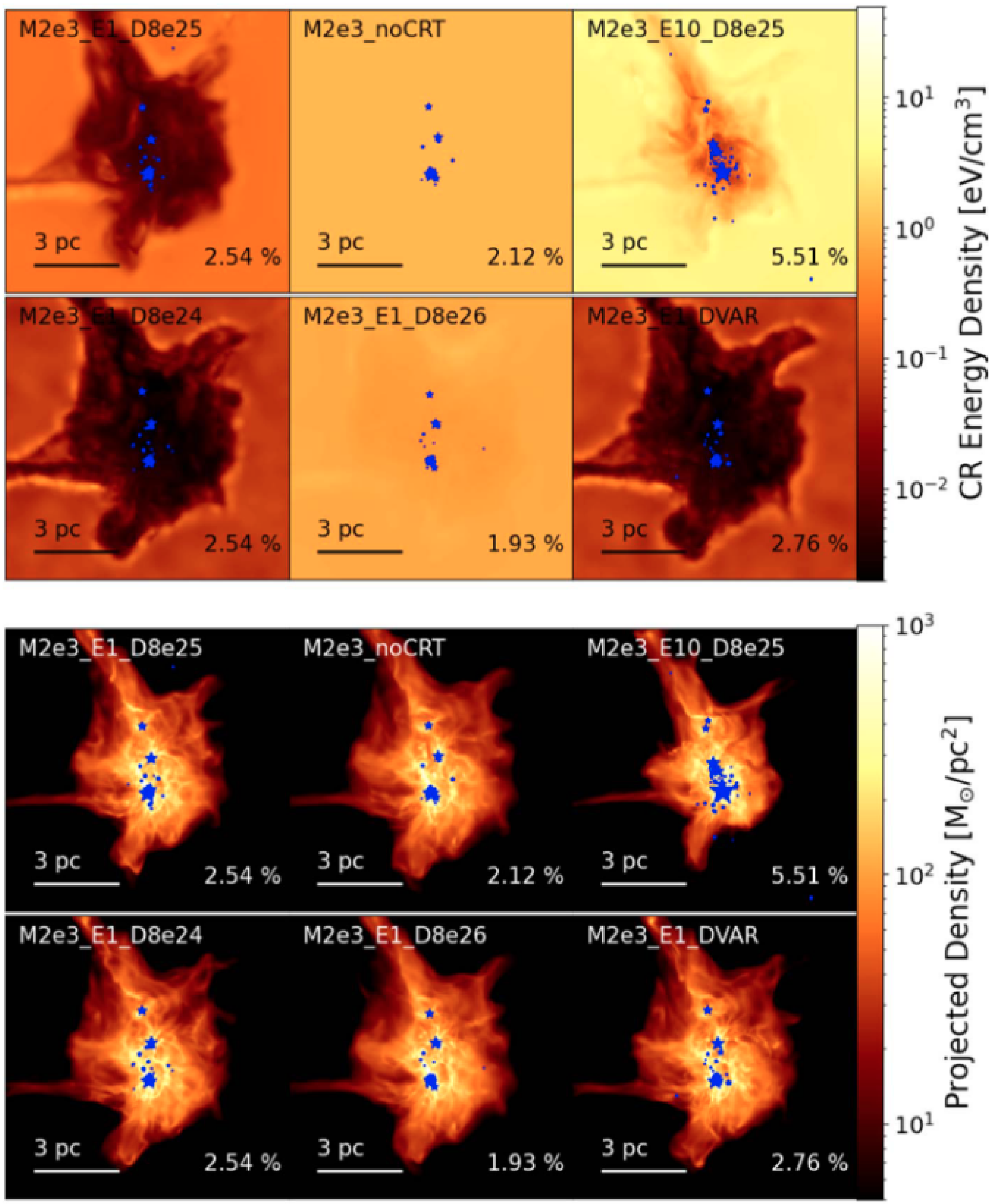

Figure 2. STARFORGE plus CRT simulation result comparison. On the upper large panel shows the CR energy density, and the lower large panel shows the projected cloud density. Six subpanels in each panel show the results with different parameters (model are named in the order of [cloud mass_CR energy density_CR diffusion coefficient]), with the upper row varying the CR energy density and the lower row varying the CR diffusion coefficient. The lower-right number shows the star formation efficiency of each model. Extracted from Figure 5 in Fitz Axen et al. (2024).

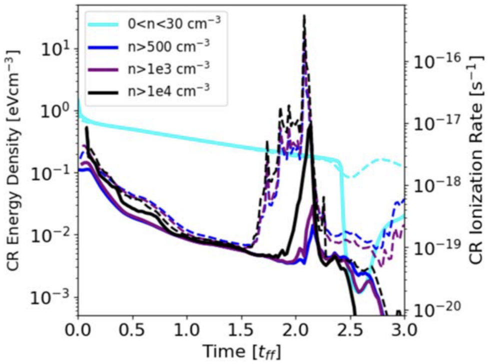

Figure 3. Median (solid) and mean (dashed) CR energy density and corresponding CRIR in the fiducial conditions ($M_{\rm cloud}$=2,000 $M_\odot$, $\epsilon_{\rm CR}$=1 eV/cm^3, $D_{||}$= 8×10^{25} cm^2/s) of STARFORGE simulation. Extracted from Figure 2 in Fitz Axen et al. (2024).

how CR transport and feedback affect abundances and ionization in dense star-forming environments.

3. SYNTHETIC OBSERVATION OF STARFORGE WITH EXPLICIT COSMIC RAY TRANSPORT

With the current state of research on CR effects in star formation, this project aims to **address a key question: How accurate are the CR ionization rates inferred from indirect CR measurements?** We aim to examine indirect (tracer-based) methods and determine whether the observed discrepancy between CRIR estimates from molecular tracers and those measured by Voyager can be explained by errors in the observational assumptions. If not, this may suggest either significant local variations in the CRIR or intrinsic limitations of tracer-based methods that may not reflect the true CRIR values.

Building on the STAFORGE simulations with explicit CRT (Fitz Axen et al. 2024), I will analyze the gas distribution in molecular clouds, model chemical evolution during star formation, and generating synthetic observations of CR tracer species. STARFORGE contains comprehensive physics in star formation, with spatial resolution spanning from cloud-scale structures down to individual stars. **By post-processing the simulations using chemical modeling, I can resolve the detailed chemistry throughout the simulation and directly compare simulated CRIR values with those inferred from synthetic observations.**

To achieve this, I will first extract relevant STARFORGE simulation properties as inputs for the chemical modeling. For each simulation cell, I will consider the following physical parameters: the gas density ($n_{\rm H_2}$), the mean cloud column density along the line of sight ($N_{\rm H}$), the gas temperature ($T_{\rm gas}$), the molecular-to-atomic H ratio ($X_{\rm H_2}$), the CR energy density ($\epsilon_{\rm CR}$), and the interstellar radiation field (ISRF). These parameters will be used in UCLCHEM (Holdship et al. 2017), or in another chemical evolution codes that best fit with our usage of modeling CR tracer species. I will **post-process fixed-time snapshots of the STARFORGE simulations with various initial conditions of CR environments through this chemical evolution modeling to produce chemical abundance maps at various evolutionary stages.** Due to the large number of required models, I will **develop a pipeline to efficiently generate, execute, store, and analyze the outputs from the chemical simulations**. Following chemical modeling, I will perform radiative transfer calculations, e.g., using RadMC3D (Dullemond et al. 2012), to generate synthetic observations of key CR tracers. These synthetic observations will enable direct comparisons between the known CRIR in the simulation and values inferred from mock and real observations.

4. PROJECT STATUS AND TIMELINE

I have completed the pipeline to extract key physical parameters from a single snapshot of the STARFORGE simulation and convert them into input files for chemical modeling. I am currently developing the pipeline which automatically runs chemical simulations for each cell. A preliminary test run on one snapshot was successful, completing approximately two million UCLCHEM simulations within two hours using the Frontera supercomputer at TACC.

The following timeline for the second-year project is as follows:

- **Summer 2025 (May-June)**: Debug the pipeline and run chemical evolution simulations for multiple STARFORGE snapshots.
- **Summer 2025 (July-August)**: Perform radiative transfer simulations, modifying an existing pipeline as needed.
- **Fall 2025 (September-November)**: Finalize radiative transfer runs, analyze results, and present progress at the Star, Planet, and ISM Seminar.
- **Winter 2026 (December-January)**: Begin drafting the paper.
- **Spring 2026 (February-April)**: Finalize the manuscript, present the second-year project talk, and submit the paper to a peer-reviewed journal before the semester ends.

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