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Executive Summary:

The resolution of the *James Webb Space Telescope* (*JWST*) has intensified the demand for high-precision astrophysical simulations to better interpret the physical processes that occur during astrophysical events. Our work primarily focuses on simulating transients, with emphasis on Type Ia SNe (SNe Ia) and core-collapse SNe (CC SNe).

SNe Ia play a critical role in high-precision cosmology and galaxy evolution, yet intrinsic variations in explosion scenarios introduce notable uncertainties. We have investigated the influence of magnetic fields on SNe Ia and found that line profiles can serve as diagnostic for constraining explosion systems. Our results also suggest that SNe Ia contribute less to the Galactic positron budget than previously assumed.

The origin of cosmic dust in the early universe remains a central question in astrophysics, as dust plays a fundamental role in shaping the evolution of galaxies, stars, and planets. While CC SNe are often cited as major dust sources, their true contribution remains uncertain. Molecular formation precedes dust formation, but the complex explosion instabilities in CC SNe causes modern forward shooting models to fail in reproducing the observed molecular signatures. To address this, we developed a novel framework that uses observations to drive radiative transport simulations, reproducing molecular spectral features in remarkable detail. This approach enables us to resolve the multidimensional structures produced by instabilities during the explosive phase of CC SNe, thereby advancing our understanding on the multifaceted physics of CC SNe and on the pathway from molecular formation to dust production.

Past Research:

Type Ia Supernovae (SNe Ia) have strong inherent diversity, arising from variations in progenitor channels, explosion scenarios, and magnetic fields. With more SNe Ia being discovered with ongoing (and upcoming) observations (e.g. ASASSN, SPECPOL, POISE, and *JWST*), its important to resolve SNe Ia through specific line profiles and analyze their role in Galaxies. The effects of positrons from SNe Ia can help with both.

Positrons are produced through the β^+ decay channel of (^{56}Ni $\overset{6d}{\rightarrow}$) ^{56}Co $\overset{111d}{\rightarrow}$ ^{56}Fe, and do not dominate energy deposition until about $\sim$ 200 days. Magnetic fields can locally contain these positrons, leading to variations in the width of line profiles, with the unblended line of FeII at 1.64 μm having been shown to distinguish some progenitor channels. We extended this previous research to find how the shape of the FeII line changes with different explosion scenarios and magnetic field shapes and strengths.

The annihilation of positrons produces a characteristic γ-ray spectrum with a prominent line at 511 keV, measured across our Galaxy. Although many sources contribute to the overall positron budget, the amount from SNe Ia has major uncertainty because their escape fraction will depend sensitively on the progenitor system. Moreover, the Carnegie Supernovae Project provides a known ratio of subluminous, transitional, and normal bright SNe Ia. Given this ratio and the yields of positrons from our models, we found that SNe Ia would contribute approximately <2...20% to the overall positron budget (compared to the current value of $\approx$ 40%), depending on the magnetic field strength, SNe Ia rate, and choice between M_{Ch} or sub-M_{Ch}.

Current Research:

Type II Supernovae (SNe II) are explosions of massive stars. SNe II with hydrogen-rich envelopes are the most common stellar explosions and are the main producers of heavy elements in the universe. As a result, the study of these cosmic explosions probes the chemical evolution of the universe, the composition of dust in our solar system, and the formation of planets. SNe II are believed to be major contributors to cosmic dust, but significant uncertainties regarding the quantity, composition, and grain size remain. The formation of molecules (CO, SiO, and more complex types (e.g. CH_3, SiO_2, SiC_2, MgO, OH, Al_2O, H_2S, ect.)) are suggested as possible pathways towards hot-dust formation due to their cooling abilities, but the complex structures found in SNe II will strongly influence both molecular and dust formation. It has frequently been shown that there are three types of instabilities that may occur during the explosive phase of SNe II. The first involves large scale mixing between stellar and explosive burning products through jet like structures. Second, Rayleigh-Taylor instabilities may mix the Si/O/C layers. Third, neutrinos may drive turbulence at the onset of the explosion. To further emphasize this point, late-time observations (> 1000 days post-explosion) consistently show clumping/caustic like structures. This leaves us with two main questions — how can the complexities between these instability types be observationally distinguished and studied, and does the formation of molecules and dust follow these structures and can we use their signatures as probes?

Commonly, molecules have been analyzed under the assumption that their features are optically thin in a

spherically symmetric, single-zone, single-temperature model. Although this quick fit technique is needed in light of the rapidly increasing IR datasets from *JWST*, it ultimately fails for the optically thick fundamental bands of CO and SiO. Detailed time-dependent radiation-hydrodynamical simulations for molecular formation would provide a more physically accurate understanding; however, these forward shooting models have been unable to match observations of the CO overtone and fundamental band by factors of 2 to 5 (see Fig. 1). This discrepancy suggests some fundamental shortcomings in how the molecules contribute to the overall temperature structure and how multidimensionality effects the molecular forming layers. A key limitation of these forward modeling approaches is their failure to resolve the complex multidimensional dynamics and the diverse hierarchy of instability scales that may develop. How, then, can we resolve the 3D morphologies in the molecular region and quantify the effect of molecules on the overall temperature structure?

To achieve this, we developed an inverse data-driven approach to analyze *JWST* spectra. Specifically, we use the observed molecular flux at a given epoch to drive non-LTE 3D radiation-transport simulations, enabling the characterization of both 3D morphologies (e.g. clumping and mixing) and molecular cooling effects by reproducing spectra with high fidelity (Fig. 1). This approach has been implemented in our newly-developed MOFAT code (MOlecular Fitting Analysis Tool), which allows us to decompose the 3D structures and temperature profile of the molecular region at a given time.

MOFAT quickly and automatically finds an optimal set of free parameters associated with the molecular features through a fixed-point iteration in a seven-dimensional parameter space. For our temperature structure, we first assume that the temperature follows the photon density. Within our molecular region, cooling by molecules is incorporated through correction factors applied to the local temperature derivatives by changes of energy at each layer. The resulting temperature profile is iterated for given parameters utilizing the flux by the overtone as an inner boundary and the emitted flux in the fundamental band as a constrain for the outer boundary. The overtone will determine the total CO mass when we have a description of the CO density distribution. We define our clumping with spheroids, whose morphology is described by three parameters: 1) the relative size of the clumps with respect to the radial dimension, 2) the density enhancement factor within the clumps relative to their surroundings, and 3) the flattening parameter of the spheroid. MOFAT assumes spherically symmetric large-scale geometry and using a solution of the radiation transport equations that include the effects of multi-dimensional clump-like structures. It takes non-LTE corrected opacities for a given chemical mixture of C, O, and Si, and then iterates all seven parameters until convergence is reached on the set that best reproduces the observations.

MOFAT is powerful in the sense that it is automatic, but it can give insight into the underlying physics and progenitors of SNe II. For SN 2024ggi, MOFAT has shown the ability to constrain the 3D fingerprints of physical processes during the explosion by tracking the time-evolution of molecular features. Between $\sim$ 300 and 400 days post-explosion, the distribution of the molecules start out almost homogeneous and then are evaporated away to expose highly clumped features. We can also constrain the chemical structures of the Si/O/C layers of SN 2024ggi — and, thus, define properties of the progenitor — by changing the chemical layout of our model and simultaneously fitting the overtone and fundamental bands of both CO and SiO. From the time series that we had with SN 2024ggi, our temperature profiles were above the formation temperature for dust. We're actively working on our analysis for: SN 2022acko, SN 2023ixf, SN 2023dbc, SN 2024ahv, and SN 2024aecx, which should begin to build a better foundation on the pathway from molecules to dust, while also letting us study the 3D structures of the molecular region and their relationship to the progenitor and the underlying explosion physics.

Future Research:

MOFATs analysis of SN 2024ggi represents a step forward in using molecules to probe the multifaceted physics of SNe II, though we have only just begun to address the main questions outlined above.

Molecular and dust formation can be separated into four distinct phases (see Fig. 2): I) the initial formation and growth of CO ($\sim$70 to 200 days after explosion), II) the early formation of SiO and, potentially, the destruction of CO ($\sim$200 to 500 days), III) the detection of more complex molecules, and IV) the rise of dust formation. For SN 2024ggi, we showed that the molecular region is continuously evolving, making the task of disentangling instabilities difficult. To separate these physical mechanisms we would require time series observations from Phase I to Phase IV — MOFAT utilizes the 'handshaking' between spectra and phases to measure the evolution and presence of structures. To date, no *JWST* observations exist for all four phases for a single SN II object. Phase I is currently missing, but it is necessary to disentangle these instability complexities through its comparisons with Phases II and III, with IV to follow suit. That said, we are actively involved in the preparation and submission of competitive proposals get these observations.

If granted, MOFAT's analysis of these observations — along with those of SN 2022acko, SN 2023ixf, SN 2023dbc, SN 2024ahv, and SN 2024aecx — will characterize the molecular and dust forming regions

in precise detail. That said, MOFAT currently includes only the molecular networks of CO and SiO. As an immediate next step, we plan to incorporate networks for more complex molecules and dust to better understand Phases III and IV. This is a straightforward process because MOFAT was built on modularity[1] and the networks for advanced molecules and dust are well known and already built for HYDRA (a radiation hydrodynamic code based out of FSU). We will have the ability to diagnose the scales of the instabilities in the molecular region, decode the pathway to dust formation, and resolve the uncertainties surrounding the influence of SNe II on cosmic dust.

MOFAT has the ability to determine the 3D structures of the molecular region of SNe II, but it currently lacks a fundamental connection to time-dependent radiation hydrodynamic simulations. Conversely, these time-dependent radiation hydrodynamic simulations lack the resolution and computational time to reproduce spectra at the pace required by the rapidly growing IR datasets. Our goal is to merge these two approaches. MOFAT will be able to map the chemical layers of the progenitor through tomography of the molecular region, bounded by the identification of hydrogen lines and explosive burning products. Additionally, MOFAT can constrain the the scales of instabilities. Together, these outputs can serve as input (or guidelines) for full time-dependent radiation-transport codes such as HYDRA or FORNAX, enabling targeted simulations from shock revival to dust formation. HYDRA is planned to be upgraded to resolve small-scale instabilities, a project I am well positioned to lead due to my expertise in domain-decomposition parallel computing. Even if HYDRA or FORNAX are unable to resolve these instabilities during my time as a postdoc, they still hold tremendous value because they can set up the initial scales of instabilities which can then be mapped to high-resolution hydrodynamic codes like FLASH. FLASH can then propagate these instabilities in a way that aligns with the scales observed by MOFAT. We will be able to trace observational signatures to the asymmetric distributions of elements in transient events.

One approach that has become popular in the SNe community is the use of templates. These templates are used to classify SNe based on spectra or to recreate light curves for cosmological distance measurements. When MOFAT reproduces a *JWST* spectra, it can take upwards of ∼1000 models to reach a converged solution. The diversity of SNe II introduces variations in molecular features, both in absolute fluxes and in the ratios between overtones and fundamental bands. Some of the 'failed' simulations found for one SN may be valid for other SNe. To address this, we aim to develop a machine learning algorithm trained on these large simulation sets to quickly identify strong starting solutions for MOFAT's fitting procedure. We are currently examining each parameter to validate MOFAT's selection process to potentially identify any degeneracies in successful fits. Once we have studied SNe II from Phases I through IV and reconstructed the progenitor scenarios as described above, we plan to incorporate time-series template matching. This method will take a time-series spectrum of a SN, fit each epoch, and identify progenitor properties as well as the type and scale of instabilities in the explosion. This is intended as future work, to be pursued after the successful completion of the tasks described above and the establishment of a robust analysis framework. Even if this stage is not reached during my postdoc, we aim to make MOFAT more accessible to the astronomical community.

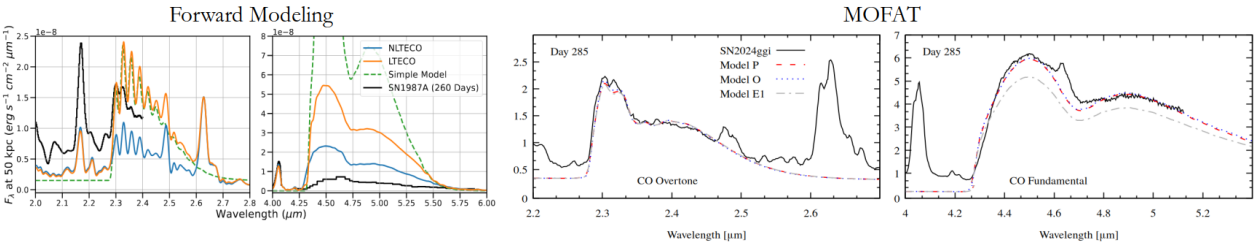

Figure 1: Comparing forward modeling methods (left, adapted from McLeod, Hillier & Dessart (2024, MNRAS, 532, 549–562)) to converged solutions of MOFAT (right). Models P and O shows prolate and oblate clumps, respectively, with Model E1 showing parameter sensitivity with slightly smaller prolate clumps.

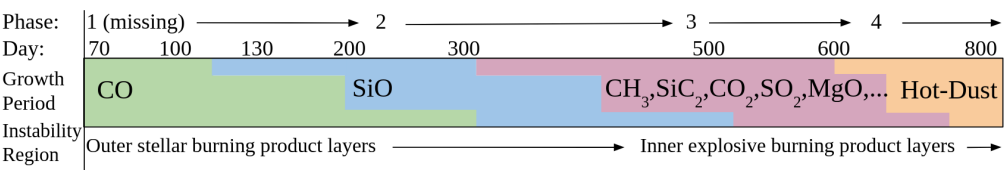

Figure 2: Graphic on the phases of molecule and dust growth and the instability region that can be studied.

[1]This modularity makes MOFAT easily adaptable to most transient events.