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EXECUTIVE SUMMARY:

We are investigating the earliest stages of cosmological structure formation—namely, the transition of the universe from a dark, empty place to one filled with stars, galaxies, and the cosmic web. In investigating the "cosmic dark ages," we focused on three specific topics: the transition between metal-free and metalenriched star formation that marks a fundamental milestone in the early epochs of galaxy formation; the evolution of the populations of high-redshift galaxies that will form Milky-Way-like objects by the present day; and the reionization of the universe by these populations of galaxies. All of these problems required simulations with extremely high dynamic range in space and time, complex physics (including radiation transport and non-equilibrium gas chemistry), and extremely large simulation volumes. We used the Enzo code, which has been modified to scale to large core counts on Blue Waters, the only machine available that satisfies the heavy data and communication needs of this best of breed study.

INTRODUCTION

The mechanisms that control the formation and evolution of galaxies are poorly understood. This is doubly true for the earliest and most distant galaxies, where observations are limited and often indirect. It is critical to understand the properties of the first generations of galaxies since they were responsible for reionizing the universe, for dispensing large quantities of metal into the low-density intergalactic medium (and thus fundamentally altering the behavior of plasmas in the future cosmological structure), and as the sites of formation and early growth for the supermassive black holes that are found at the center of every massive galaxy at the present day. Understanding the first generations of galaxy formation-the goal of this research projectis critical to the interpretation of current and future surveys of both the most distant galaxies that can be observed and also of our own Milky Way. More generally, this work helps to answer the philosophical questions "where do we come from?" and "how did we get here?"

METHODS & RESULTS

Our simulation tool of choice is the Enzo code [1,2], an open-source, community-developed software platform for studying cosmological structure formation. Enzo allowed us to include

all of the critical physical components needed to study galaxy formation—gravity, dark matter dynamics, fluid dynamics, the microphysics of plasmas, and prescriptions for star formation and feedback—and to do so using a tool that can scale to large numbers of CPUs. All analysis was done with the YT code [3,4].

Using Blue Waters, we successfully modeled the formation of the first generation of metalenriched stars in the universe and showed that there are several possible formation modes for these stars. These included self-enrichment of the halo where the first primordial star formed and pollution of neighboring halos by the supernova remnant. In addition, we showed that the presence of dust (which may form in the ejecta of the first supernovae) can have a critical effect on metal-enriched star formation, directly resulting in additional cooling and the formation of additional molecular hydrogen. Extra hydrogen further increases cooling rates and may cause additional fragmentation and lower-mass stars.

We have also modeled the evolution of large populations of galaxies in the early universe in several different large-scale environments. We find that if these Population III stars form massive black hole/stellar binary systems, they are likely to be prodigious emitters of X-ray radiation. This radiation both heats and ionizes the intergalactic medium, in some cases to 10⁴ Kelvin! This may be important for predicting the topology of the 21 cm neutral hydrogen signal, which will be detectable by low-wavelength radio arrays in the coming years. We also show that radiation from early star formation can help suppress the collapse of gas in neighboring halos, delaying star formation and causing the galaxy luminosity function to be strongly suppressed at lower luminosities.

WHY BLUE WATERS?

To properly model the earliest galaxies, our simulations required complex physics—most importantly, radiation transport and nonequilibrium gas chemistry—and extremely high spatial and temporal dynamic range. Furthermore, large simulation volumes (and thus many resolution elements) were needed in order to model enough galaxies to be able to adequately compare theory to observations in a statistically meaningful way. Taken together, this required the use of a supercomputer with large memory and disk space (to accommodate the tremendous dataset sizes), large computational resources, and an extremely high-bandwidth, low-latency communication network to enable significant scaling of the radiation transport code. Blue Waters is the only machine in the U.S. available to the academic community that fits all of these requirements.

Given the expected increase in machine size for the next Track-1 system, we will be able to expand our research in several dimensions: we will be able to increase our simulation spatial resolution by at least a factor of two and mass resolution by a factor of ten, which will enable us to explore even fainter galaxies than we are currently examining; we will be able to extend our simulations to later times, thus making a wider variety of useful predictions (i.e. we will be able to predict galaxy properties for both groundand space-based telescopes, as opposed to solely space-based telescopes); and we will be able to include additional physics, such as active galactic nucleus feedback, that is not currently in our models.

PUBLICATIONS

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FIGURE 1

(BACKGROUND): The gas ejected from the supernova created by the first star to form in a cosmological volume as it is leaving the dark matter halo where the star formed. The supernova remnant preferentially expands into the void regions near the halo rather than the filaments, since this is the path of least resistance, and fills the intergalactic medium with metal-enriched gas. Simulations first published in Smith et al. (Astrophys. J., submitted).