<u>**Figuring Out Gas & Galaxies in Enzo (FOGGIE): The Gas-Galaxy Connection at *z*>2**</u>

Figuring Out Gas & Galaxies in Enzo (FOGGIE): The Gas-Galaxy Connection at z>2

We request 3 years of funding, primarily to fund two postdocs for 4 cumulative years, to address the unsolved problem of galaxy feedback by providing a major step forward in our ability to analyze the connection between galaxies and their circumgalactic gas. We propose (1) a new set of cosmological hydrodynamic simulations of unprecedented resolution, (2) a novel refinement scheme for achieving this resolution, (3) synthetic observations of simulation data and an open-source pipeline for producing mock data from other simulations, and (4) a novel approach to varying feedback recipes and assessing their effects on observable data of both stars and gas.

1. The Big Picture: the Baryon Cycle, Feedback, and the Gas-Galaxy Connection at z>2

1.1 The current landscape and future prospects: The ways in which galaxies acquire, process, enrich, and expel their gas—known as the "baryon cycle"—are among the most complex and important processes in astrophysics. Inbound flows, driven mainly by gravity and cooling, transport gas from the intergalactic medium (IGM), through the circumgalactic medium (CGM), into the interstellar medium (ISM) where it forms stars, feeds AGN, and is enriched by heavy elements. Outbound flows are driven by supernovae, AGN jets, and radiation that push enriched gas and dust back to the CGM and beyond, perhaps to be recycled. Inside galaxies, inflowing and recycled gas fuel star formation, while feedback heats the ISM and drives outflows, regulating or quenching star formation. Intense attention over the last decade has revealed that, at least at z<1, the CGM is a major component of galaxies (see Tumlinson, Peeples, & Werk 2017 for an up-to-date review). Existing simulations provide a good foundation for interpreting the observational results, using the mass, kinematics, metallicity, and evolution of the CGM and galaxies to constrain the mechanisms of feedback that are so critical to galaxy formation.

We anticipate rapid progress in observational studies of the gas/galaxy connection at the z>2 epoch, owing to the growth of ground-based spectroscopic datasets and future facilities. *JWST* will reach much deeper into the galaxy population, and to much higher redshifts, than has been possible to date, drawing a richer picture of this connection when added to the already large body of ground-based spectroscopy of the gas. *JWST*'s deep spectra at 1–20 micron and un-obscured views of galaxy morphologies will supply the galaxy side of the gas/galaxy equation, offering a new window into the important physics and drawing solid links to *Hubble*'s work at z<1. Fully interpreting these new data, however, will require new theoretical models, synthetic observations, and analysis methods: FOGGIE will explore both the physical *and* observable effects of feedback on z>2 galaxies.

To address the baryon cycle at z<1, our group has developed novel approaches to simulating the gas-galaxy connection and synthesizing mock data. We have achieved $10^{4\text{-}5}$ times finer mass resolution in galactic gas flows than conventional cosmological simulations, and we are developing new tools for making synthetic data. We propose to apply these new techniques at z>2, when star formation and black hole accretion rates were rising (A. Hopkins et al. 2006, P. Hopkins et al. 2007), when the potential impacts for feedback on the baryon cycle are strongest, and where data expected from *JWST* will revolutionize our empirical view of these galaxies. *Our main scientific goal for this work is to understand the CGM and ISM gas processes that govern star formation and morphology in observable ways.*

1.2 Suitability for ATP: The Astrophysics Theory Program is the natural source of support for this work. Our goals are consistent with NASA's strategic Objective 1.6 to "Discover how the Universe works. . . ";. We will provide physical models and synthetic data for comparisons to observations from current and future NASA facilities such as *Hubble* and *JWST*. Our broad program surpasses the scope and funding scale of the *Hubble* theory program. With *JWST* set to be commissioned for science by Spring 2019 (before the next ATP deadline), it is important that we begin this work *now*.

1.3 This proposal: This proposal centers around four inter-related science questions:

(1) Stars: How do feedback, accretion, and gas recycling affect resolved star formation histories?
(2) ISM: How do star formation and AGN feedback affect the physical properties of the ISM at z>2, and what diagnostics accurately trace these properties?
(3) CGM: How does feedback affect the physical and observable properties of the CGM?
(4) Metals: How does feedback affect galactic metal budgets and metallicity scaling relations?

We will address these important questions with a novel combination of extreme resolution in the gas flows around galaxies, a suite of synthetic data, and new treatments of stellar and AGN feedback.

Resolving the baryon cycle: Constraining physics with observations usually requires resolving scales smaller than what can be directly observed. Conventional galaxy formation simulations generally strive for physical resolutions of <100 pc but have >1kpc or larger resolution in the low-density CGM. Hence CGM mass resolution for most simulations is still 10^{4-5} $M_\odot$ and often 10-100x worse, with little emphasis (or CPU hours) on this phase. We have extended the Enzo hydro code (Bryan et al. 2014) to reach spatial resolution of ~10pc and mass resolution down to 100$M_\odot$ in the CGM. Our tests show CGM resolution has major effects on convergence in the physical and observable results.

The importance of synthetic data: Simulations track physical conditions (temperature, density, angular momentum, etc.) as a function of time, but observations capture single still-frame snapshots of the light from stars or gas modulated by dust, viewing angle, wavelength, surface brightness dimming and instrumental effects. Connecting *light* back to *physics* is non-trivial. It is *only* with synthetic data—with pixelization, noise, PSFs, artifacts, etc., akin to real data—that we can reach insights about the *real* observed universe. We will release all our pipelines as open-source code; likewise, all data products will be released to aid observers proposing or analyzing similar data.

Understanding the physical impact of feedback: This is a key goal, which we will address by refining Enzo's subgrid star formation and AGN feedback prescriptions at the increased ISM and CGM resolution. We will also use a novel "flux tracking" technique that correlates outcomes, such as CGM mass density, temperature, and metal profiles against the robustly measured inputs to the CGM—mass, heat, and entropy—which further sharpens the physical relationships of interest.

We describe our simulations and synthetic data in §2 and how we will use the FOGGIE simulations to address our four science questions in §§3 to 6, respectively. We conclude in §§7 and 8.

2. Figuring Out Gas & Galaxies In Enzo (FOGGIE)

This section describes our simulations' galaxy and feedback properties (§2.1), our novel refinement scheme (§2.2), our new astrophysics modules (§2.3), and our synthetic data pipeline, MISTY (§2.4).

2.1 Simulation suite: Our production runs will evolve ~25 halos to z=2 using a novel forced-resolution scheme to capture the small scales relevant for the evolution of both the ISM and CGM. Host dark matter halos will be chosen at z=2 out of a 100 cMpc/h volume based on their mass, environment, formation history, and spin, and will be re-simulated with MUSIC (Hahn & Abel 2011) to yield our initial conditions. We will select 5 "low mass" halos (~0.1 L^*), 15 ~L^* halos with a range of halo assembly times, and 5 of the most massive halos in the volume. We will adopt state-of-the-art star formation and feedback algorithms, prescriptions for AGN feedback, and non-equilibrium primordial and metal-enriched chemistry and cooling. Most critically, the production runs will use a novel "forced refinement" scheme to resolve the CGM at unprecedented spatial and mass resolution (see §2.2). *No extant simulations can adequately address our science goals.*

Recent work demonstrates that sub-grid models for star formation and AGN feedback are among the most critical, and yet poorly understood, ingredients in resolving the properties of galaxies

(Scannapieco et al. 2012, Kim et al. 2016, Schaye et al. 2015, Naab & Ostriker 2017). Enzo has a variety of stellar and AGN feedback algorithms already implemented, and more are in development (§2.3). Our simulations will explore the dependency of the results on these feedback algorithms, by exploring different stellar and AGN efficiency and feedback (such as Sedov-like kinetic feedback, cosmic ray and magnetic field injection, and pre-heating of the gas by OB associations, see §2.3).

We expect to do the largest parameter search on a small number of halos, applying our most promising feedback schemes to the other halos in the FOGGIE suite. In order to avoid missing non-linear couplings between model parameters, we will typically not manipulate a single parameter at a time; rather we will vary multiple parameters in many of our simulations simultaneously, and will use Gaussian process emulation (see, e.g., Gómez et al. 2012, 2014) to disentangle the relationship between simulation inputs (including not only parameters for star formation and feedback but halo mass and formation history) and observational characteristics of these galaxies. Comparisons between these simulations and data at z=2 will enable a similar, future feedback study at z<2 by narrowing the parameter space for which simulations need to be evolved to z=0.

2.2 Forced refinement for fine galactic and circumgalactic resolution: A key part of our simulation strategy exploits a novel capability of adaptive mesh refinement (AMR) simulations: the ability to resolve regions of the calculation to arbitrarily high spatial and temporal resolution. Rather than following the standard Lagrangian-like refinement typically used in AMR cosmological simulations (where the mass of gas and dark matter in a resolution element are kept roughly constant by iterative refinement), we will ensure that the CGM around our galaxies is always refined to very fine *spatial* resolution in a sphere centered on the galaxy's center of mass (see Figure 2 for an example). This "forced refinement" allows us to apply extremely fine mass resolution even in the low density gas of the CGM and accurately capture heating, coooling, and condensation at the relevant small scales while retaining the full cosmological context of the simulation. We plan to force refinement down to

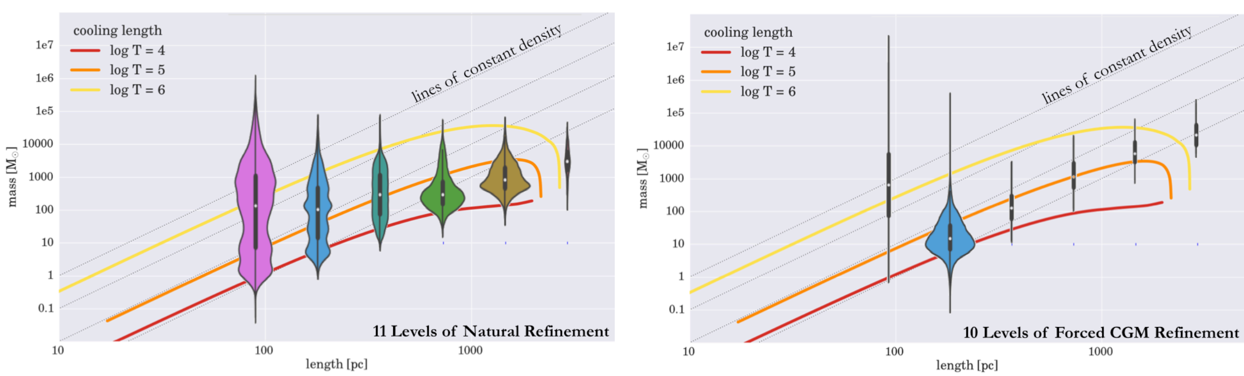

Figure 1: Resolution and cooling length at z=2. The thin dotted lines are lines constant density; the colored lines are the cooling lengths for different mass scales and temperatures with a Haardt & Madau (2012) EUVB for CGM densities at z=2 (here, $<10^{-23}$g cm^{-3}) at 0.1$Z_\odot$, calculated using Grackle (Smith et al. 2017). The cooling length ($t_{\rm cool}\times c_{\rm sound}$) sets a natural fragmentation scale: gas at this scale will cool and condense into smaller clouds. The "violin" wedges denote the distribution of AMR cell sizes and masses in a naturally-refined run (resolution set by the local density) and in a forced-refinement run; the cell size discretization owes to the factor of 2 decrease in cell size with increasing levels of refinement. (As there are more than 200 times as many cells in the forced refinement run as in the natural refinement run, the total number of $n_{\rm ref}$=11 cells is comparable.) Our production runs will resolve the CGM to a factor of 2–4 smaller scales than in this test run, allowing the CGM to naturally fragment and cool; by forcing the refinement to be at a small scale throughout the CGM, essentially *all* circumgalactic gas will be adequately resolved.

27-54 physical parsec out for the disk and star formation (out to R ~10 kpc), to 50–100 physical pc out to ~$0.5R_{vir}$ and 100–200 physical parsec out to ~R_{vir}. At CGM densities these cell sizes correspond to a mass per cell of $10^{2\text{-}3}$ $M_\odot$ (Figure 1). This resolution in the halo ensures that the cell sizes are much shorter than the gas cooling lengths (Figure 1)—guaranteeing we capture the thermodynamic evolution correctly. For a few cases, we will increase the resolution by another level of refinement in order to demonstrate convergence. (We are separately exploring the effects of resolution alone on the low-redshift CGM as part of HST AR #15012 [PI Corlies, Co-Is include Peeples, Tumlinson, and O'Shea].)

We emphasize resolution in the low-density gas to support our main science goal of understanding how flows in the CGM and ISM influence galaxy star formation and morphology (and vice versa). Given finite computing resources, this choice means we cannot simulate large volumes and statistical samples of galaxies at uniform resolution (e.g., Illustris; Suresh et al. 2015) or apply extremely high resolution to the ISM and star formation all the way to *z*=0 (e.g., FIRE and Latte; Wetzel et al. 2016). Even in runs where the mass resolution approaches the high end of what FOGGIE will achieve (e.g., Eris, the EAGLE zooms, and Latte reach $10^{3\text{-}4}$ $M_\odot$ for *single* particles), the spatial resolution in the CGM is only at the kpc scale because of smoothing and hinders the ability to

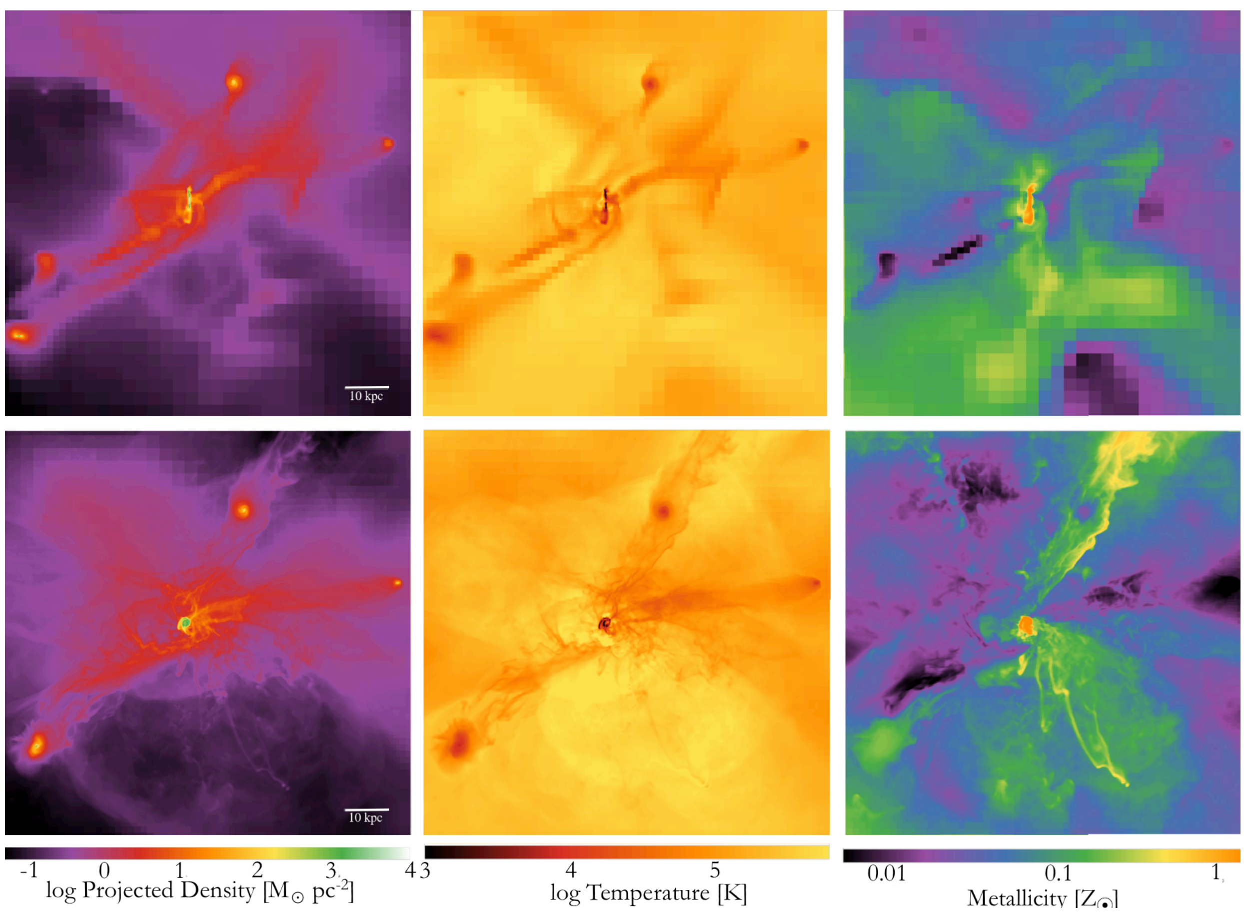

Figure 2: Projections of density, temperature, and metallicity in traditional "natural" refinement (top) versus our new forced refinement scheme (bottom) at *z*=2. The properties of both the CGM and the galaxies are dramatically altered *with no changes whatsoever to the underlying feedback recipe*. Both models have natural refinement to down to 100 pc (n_{ref}=11), while the forced refinement run has 200 pc cells (n_{ref}=10) in the CGM, the *coarsest* CGM resolution our proposed suite will have.

correctly follow the evolution of a multi-phase CGM. No matter how sophisticated the subgrid feedback or cooling models, conventional simulations with any of these codes stand a very strong chance of *significantly* under-resolving the physics of the CGM because they do not emphasize small particles or high refinement in low-density gas. Due to the fixed gas and dark matter mass resolution of particle-based codes, this is a limitation that is extremely difficult to overcome. Other researchers using grid-based codes could in principle reproduce our technique, but no such results have been published. Thus FOGGIE occupies its own niche in the simulation ecosystem, where it is optimzed for relating CGM and ISM gas flows to resolved galaxy star formation and morphology.

2.3 A major piece of this work will be code development relevant to galaxy evolution.

Deliverables: improvements to the open-source Enzo and Grackle codes

1. *Star formation feedback improvements*: Enzo already includes thermal, kinetic, and cosmic ray feedback from supernovae, but does not yet include the earlier stellar winds or radiation pressure from massive stars. Massive star feedback clears out the dense gas of star forming regions (e.g., Lopez et al. 2011), allowing fresh supernova ejecta to escape galaxies and helping to suppress star formation (Hopkins et al. 2014, Muratov et al. 2015). We will also ensure supernova energy feedback consistent with a chosen IMF and modern stellar evolution calculations. The level to which massive star and supernova feedback couples to the surrounding ISM (27 cells surrounding a star particle; Simpson et al. 2015) will be one of our primary feedback "knobs".
2. *AGN feedback improvements*: Enzo features several ways to model feedback from supermassive black holes, including jet-based, thermal, and radiative feedback. As the underlying physics of AGN feedback is *extremely* uncertain, we will employ multiple models. The simplest assumption is local thermal feedback triggered by cold, dense gas, but this results in unphysical behavior in galaxy clusters (Li et al. 2015, Gaspari et al. 2014, 2015), although such a feedback mechanism is possibly more appropriate in $z{\sim}2$ L^* galaxies. We will experiment with jet-based feedback, which is likely to deposit more energy in the CGM than in the disk. A hybrid method also exists, with feedback energy split between thermal and kinetic feedback (Meece, Voit & O'Shea 2016). These methods are computationally costly, but since we only need to evolve the simulations for roughly 3 Gyr they are tractable using the requested NASA HEC resources. How AGN couple with their environs will be our other main feedback knob, primarily in the most massive halos.
3. *Chemical evolution improvements*: Enzo currently only tracks a single "metal" field in addition to H, H_2, and He. We will implement new tracers for carbon, nitrogen, oxygen (and other α-elements), iron-peak elements, and r- and s-process elements. These will trace contributions from Type II supernovae, Type Ia supernovae, AGB stars, and compact remnant mergers.
4. *Cooling improvements*: Enzo's cooling module, Grackle (Smith et al. 2017), includes non-equilibrium abundances of hydrogen and helium, but assumes ionization equilibrium (and the resulting cooling rates) from metals with Solar abundance ratios. We will improve Grackle to include multiple-element cooling as in Wiersma, Schaye, and Smith (2009) and the effects of non-equilibrium chemistry for important metal species using, e.g., Dengo or Krome.

2.4 The MAST Interface to Synthetic Telescopes with yt (MISTY):

Deliverables: pipelines for generating synthetic data; mock galaxy images and spectra for *Hubble* and *JWST* and mock CGM absorption spectra, with associated physical parameters

Enabled Science: synthetic data for other facilities (*WFIRST*, *LUVOIR*, X-ray observatories)

Constructing and analyzing synthetic data at a high degree of realism is central to our program, and is driven by the need to provide ever-more-precise comparisons between simulations and observations in order to most effectively inform and falsify models. We will build synthetic data pipelines in Python, using the open-source analysis software yt (Turk et al. 2011) as its starting point: yt is highly modular, so the MISTY pipeline easily port any other simulation evolved with a code yt supports (essentially all major astrophysical hydrodynamics codes). We will release our mock data and the pipelines for generating them via the Mikulski Archive for Space Telescopes (MAST) at STScI and Github (respectively). The construction of these search interfaces is separately funded (HST AR #13919, PI Peeples); *no funds from the proposed program will go to MAST*. By including our synthetic data in MAST, the extensive suites of mock images and spectra *and associated physical parameters* will be easily searchable by the community. For example, one will be able to search our suite of mock images by either galaxy stellar mass or by "observed" JWST NIRCam/F277W magnitude, or the suite of mock CGM absorption spectra by either the metallicity of an absorber and by the "observed" O VI equivalent width. This direct linking enables easy predictions for proposals and subsequent data analysis.

We will construct several modes of synthetic data for a variety of NASA observatories and instruments in order to address each of our science goals:

(1) **Images** – Galaxy morphologies and sizes (§3): *Hubble* WFC3/IR, *JWST* NIRCam. Galaxy masses: *Spitzer* IRAC. CGM emission: Keck/KCWI, *LUVOIR*'s HDI.
(2) **IR low/moderate resolution spectroscopy** – ISM emission-line patterns, AGN (§4): *Hubble*'s WFC3/IR, *JWST*'s NIRSS, *WFIRST*'s WFI/grism.
(3) **IR moderate resolution spectroscopy** – Galaxy dynamics, ISM properties (gas-phase metallicities, shocks/ionization, star formation rates), AGN (§§3, 4, and 6): *JWST*'s NIRSpec & MIRI, Keck's OSIRIS and MOSFIRE, *LUVOIR*.
(4) **UV & Visible high resolution spectroscopy** – CGM absorption (§§5 and 6): Keck's HIRES, *LUVOIR*'s LUMOS and ONIRS
(5) **X-ray** – AGN properties (§3): *Chandra, Lynx*.

Our top priority and key deliverables will be *JWST* and *Hubble* data for the galaxies and Keck's HIRES data for CGM absorption. However, given an instrument model, the MISTY pipeline will enable synthetic data to be straightforwardly generated for the other instruments listed above as time and community interest allows.

We will construct synthetic data for galaxies using the radiative transfer Monte Carlo ray-tracing code Sunrise (Jonsson 2006), including the effects of viewing angle, dust, and other software our group will develop as needed. Our group has extensive experience synthesizing publicly available tools such as stellar population models (Conroy 2013), Cloudy (Ferland et al. 2013), and MAPPINGS (Allen et al. 2008) to create and analyze both mock images and spectra (e.g., Snyder et al. 2011, 2015; Ford et al. 2016); see examples in Figures 3 and 6. We will construct high spectral- and spatial-resolution, idealized predictions for the SED of our galaxies before they would enter a telescope. These synthetic galaxy data cubes, on which the images and galaxy spectra will be based,

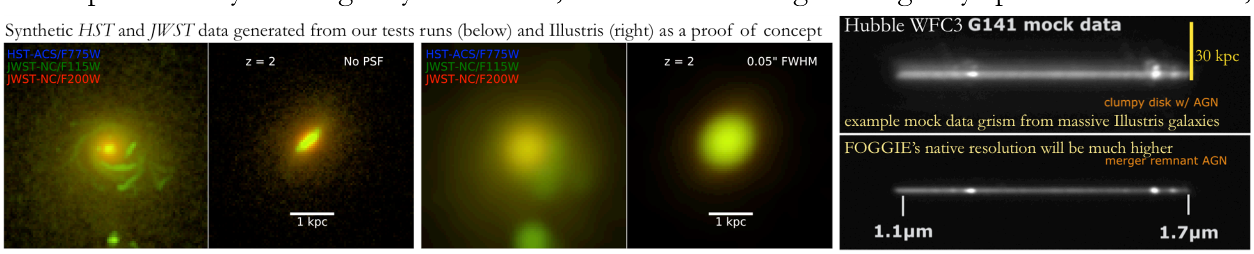

Figure 3: Example synthetic data at z~2. Left: our code for mocking *Hubble* and *JWST* images applied to our test case of a dwarf galaxy in a natural vs. forced refinement runs (cf. Figures 2 and 5); only approximate PSFs and no astronomical noise or detector effects have been applied. CGM resolution alone dramatically alters the observed morphology. Right: our code for generating mock grism data applied to two massive galaxies from Illustris; note that the FOGGIE simulations will have *much* finer ISM resolution and less massive dark matter and stellar particles than in Illustris.

will include (1) stellar emission from publicly available stellar population synthesis models; (2) HII region emission based on either the young stellar particles (e.g., Kewley et al. 2001; Groves et al. 2008) or the native gas properties (e.g., Cloudy); (3) AGN emission, including the narrow-line region, based on the simulated SMBH accretion rates (e.g., Heckman et al. 2004, Groves et al. 2004, Hopkins et al. 2007), and (4) the effects of dust (generically simple "Milky Way" or "SMC"-like dust, though our separately-tracked elemental abundances will enable more complex models (e.g., Draine 2003). From these data cubes, we will apply instrument simulation software appropriate for the science goals of each project, typically including convolution with point-spread and line-spread functions, binning to instrument sampling scales, and the addition of dominant noise factors such as sky shot noise. These data cubes, with and without instrument simulations applied, will be our primary deliverables to MAST. With the associated *physical* galaxy properties intrinsic to the simulations, these synthetic data will enable a deeper analysis of real data than simpler models.

For CGM absorption, the MISTY pipeline uses Trident (Hummels, Silvia, & Smith 2017), which we will adapt for Keck's HIRES spectrograph (see Figure 6). Trident calculates ionization fractions and then the optical depths as a function of position and velocity along a given sightline; the MISTY pipeline then delivers both the high-resolution, noiseless intrinsic spectra and associated physical parameters (density, temperature, metallicity, ionization fraction, kinematics, etc.) and the observed absorber column densities, equivalent widths, etc., along with absorber-weighted physical properties. In addition to the metagalactic UV background, we will include self-consistent sources of local radiation, including the galaxies' AGN. Directly coupling observations to physical processes will inform interpretations of both ground- and space-based observational campaigns, enabling forecasts of the observational capabilities of future space missions such as NASA's *LUVOIR* Surveyor mission concept. All these products will be publically released via STScI's MAST archive.

3. The stars: tracers of galaxy assembly

Deliverables: idealized and "observed" synthetic images and resolved spectra, non-parametric morphology measurements
Our Science: effects of feedback & accretion flows on resolved star formation histories
Enabled Science: effects of feedback on sub-kpc-sized star cluster luminosity distribution, merger morphologies, AGN host galaxy selection effects, feedback models to test to z=0

3.1 Star formation regulation and morphological transitions: Large *Hubble* imaging (e.g., COSMOS, Scoville et al. 2007, and CANDELS, Grogin et al. 2011), and low-resolution spectroscopy (3D HST, Momcheva et al. 2016) surveys have revealed galaxies at z>2 are morphologically more diverse than their descendants (Bruce et al. 2012), often with bright off-center luminous star-forming regions (unresolved "clumps", Guo et al. 2015). The distribution of these regions is sensitive to how feedback (Moody et al. 2014) and disruptive events (such as mergers) heat and drive turbulence in the ISM (§4), and, perhaps, to how galaxies acquire gas from the CGM and IGM (§5). Meanwhile, angular momentum exchange with the halo (Bullock et al. 2001, Dekel et al. 2009, Genel et al. 2015) conspires to turn these lumpy z~2 galaxies into the rotationally supported disks common at z<1. **With *JWST* we will, for the first time, have spatially-resolved star formation histories for large samples of high-redshift galaxies.** While the regulation of star formation—how gas accretion and feedback balance—is at the core of any galaxy evolution model, we are interested in how this gas-galaxy connection manifests in both the rates and morphologies of star formation at the time when the correlations between structure, star formation, and stellar mass seen today first emerged (e.g., Wuyts et al. 2011, Figure 4).

While it is unlikely even one of the most massive halos in our 100cMpc/h box *should* quench by z=2, we will track the beginnings of the formation of massive, compact bulge-dominated galaxies (van

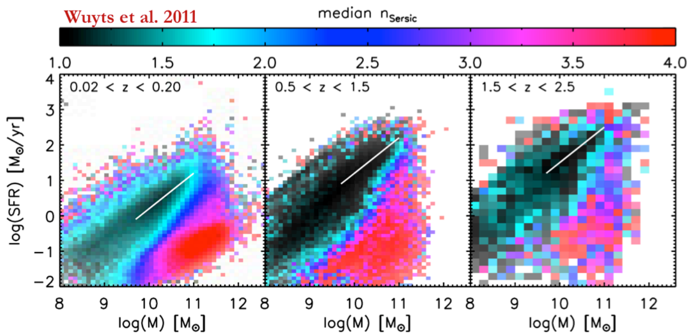

Figure 4: Galaxy morphologies are correlated with their star formation rates at all redshifts.

Dokkum et al. 2008) that have been linked with the quenching of star formation. Proposed mechanisms for how galaxies quench all rely on the gas-galaxy connection, as either galaxies cease forming stars from their gas or they cease *acquiring* gas from the CGM with which to form stars—yet *no* extant simulations adequately resolve these flows. With our superb circumgalactic resolution, we will test how halo accretion shocks affect galactic accretion rates and subsequent star formation ("mass quenching", Lilly & Carollo 2017). Varying star formation and AGN feedback strengths, we will test how injecting heat and momentum into interstellar gas drives violent disk instabilities and compaction (Ceverino et al. 2014; Porter et al. 2014, Zolotov et al. 2015). As no simulations have managed to self-consistently "solve" quenching, we do not set that as our aim; rather, we will fully explore how circumgalactic gas flows and feedback modify galaxies' resolved star formation histories. In our lower mass halos, resolving circumgalactic flows may help solve the over-efficiency with which high-z dwarf galaxies form stars from gas accreted onto the halo (White et al. 2015).

3.2 Star formation histories *<u>are</u>* *the history of galaxies' gas*: FOGGIE will uniquely address morphological and star formation transitions by tracing the questions of how energy and momentum injection into the ISM affect subsequent episodes of star formation while simultaneously resolving the gas flows into and within the halo. Galaxies' star formation histories, how current star formation is distributed through the disk, kinematics, and structure are all influenced by circumgalactic gas flows. This can be seen in the resolution comparisons with and without forced refinement, as rendered into mock images of stars, in Figure 3. Strikingly, not only did the morphology but also the *orientation* (and hence angular momentum) of our test case galaxy change (Figures 2, 3, and 6) *with only changing how finely the CGM is resolved*. The star formation histories in the two runs, while broadly similar, also differ in the details: the refined galaxy is ~20% more massive, owing to a couple of extra starburst episodes since z=4 that the naturally refined galaxy did not experience.

We also expect our forced refinement scheme to impact how minor mergers deliver gas to galaxies. Most galaxies accrete few stars through numerous minor mergers, but these mergers should deliver rich gas reservoirs, potentially driving not only spheroid formation but also disk formation (e.g., Robertson et al. 2006, Snyder et al. 2015). In our test cases, however, gas stripping of infalling satellites is strongly affected by how finely the CGM is resolved (see Figure 6). Therefore, in order to determine how these processes assemble the galaxy structures we observe, it is critical to accurately trace the flow of matter in the simulated galaxies' halos (§5). Our feedback parameter studies will place interesting constraints on the heating rates and timescales on which feedback affect the morphologies and rates of star formation in a fully consistent gaseous halo.

3.3 Synthetic data is key to comparing theoretical and observed resolved star formation histories: Even in *JWST*'s resolved star formation histories, there will still be structure below *JWST*'s resolution; with our mock images and spatially-resolved spectra, we will test how the effects of feedback *observable* galaxy properties. Galaxy morphologies and structural parameters all depend on the wavelengths at which they are measured; by comparing *true* galaxy dynamics and ones filtered through *k*-corrections in our mock images, we will more robustly interpret *JWST* observations. Synthetic galaxy data are also crucial for testing measurement methods, such as the extent to which star formation histories (and stellar metallicities, §6) are biased by younger and more luminous stars.

4. The interstellar medium: shocks, turbulence, dust, AGN, and emission lines

Deliverables: synthetic spectral cubes covering common diagnostic lines, realistic mock spectra and line maps for *JWST* and *Hubble*, line flux and velocity measurements

Our Science: effects of feedback on ISM properties and emission line ratios and diagnostics

Enabled Science: optimized diagnostics of AGN emission versus ISM shocks, the connection between observationally selected AGN and their host galaxies**,** effects of feedback on dust properties, molecular gas predictions (ALMA, warm H_2 for *JWST*)

4.1 Interstellar gas at z>2: Star formation rate surface densities are generally much higher at *z*>2 than in the local universe, suggesting that either *gas* surface densities are likewise higher, that star formation rate efficiencies are higher, or both. Recent observations with ALMA and other observatories have found molecular gas fractions to be fairly high (Carilli & Walter 2013, Scoville et al 2017). Combined, the empirical picture of interstellar gas when cosmic star formation rates and AGN activity peaked is one of mergers and winds shocking gas and driving turbulence, yet stars efficiently and quickly forming out of relatively dense but highly excited gas. We are interested here in the physics and observability of the baryon cycle *within* these galaxies: how does feedback regulate star formation, i.e., how does accretion from the CGM and radiation, energy, momentum injection from massive stars, supernovae and AGN impact the physical properties of interstellar gas, thereby driving galactic winds (or not) and potentially affecting the ability of the gas to cool and form stars?

4.2 Emission lines as diagnostics: Flux ratios of strong optical emission lines have long been used to characterize the physical conditions of HII regions, AGN, and the galaxies in which they reside (Baldwin, Phillips, & Terlevich [BPT], 1981; Kewley et al. 2006). The physical conditions of the ISM (density, temperature, ionization state, etc.) are both intrinsically interesting as markers of star formation and AGN feedback, but also necessary inputs to measuring ISM elemental abundance ratios (e.g., O/H, N/O, §6). Sometimes these properties can be estimated directly from the spectra: lines that trace temperature (e.g., [OIII]λ4363, [NII]λ5755, and other auroral lines), density (e.g., [SII]/Hα), ionization (e.g., [OII]/[OIII]), but for any given galaxy, these lines are not always bright enough or necessarily in the bandpass of interest. The incident radiation field must also generally be assumed, from a combination of stellar population synthesis models and AGN templates, as (in the absence of X-ray data) the emission line ratios (e.g., [OIII]λ5007/Hβ or [OI]λ6300/Hα) are often used as a sign of AGN activity or a lack thereof. Each of these physical properties should change at higher redshift: younger, more metal poor stellar populations (Levesque et al. 2010) and more abundant AGN harden galactic radiation fields, and the ISM is generically denser, but also hotter, than at *z*~0.

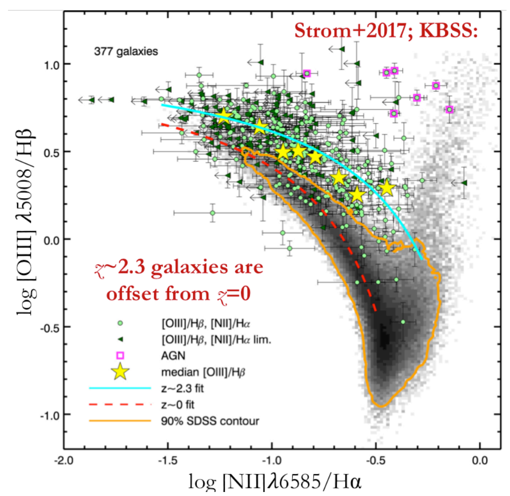

Figure 5: The emission line ratios of ISM of *z*>2 galaxies are offset from where *z*=0 lie

Measuring emission line ratios in high-redshift galaxies will be a high-impact use of *JWST*, as at *z*>2 the relevant emission lines shift into the infrared, competing with water in the Earth's atmosphere in order to be observed from the ground. Despite these challenges, ground-based observations reveal galaxies in the early universe to have emission line ratios in different portions of diagnostic space than their low-*z* counterparts (e.g., Shapley et al. 2015, Strom et al. 2017, Figure 5), signifying interstellar physical conditions do evolve with time. In particular, (§6) ISM metallicities are generically lower at earlier cosmic times, though quantifying metallicity evolution relies intimately on how diagnostic line ratios (e.g., R_{23}, [OIII]/[NII], and [NeIII]/[OII], Maiolino et al. 2008, Shapley et al. 2017) depend on *other* ISM properties (Kewley et al. 2013). Further complicating conversions from line emission to gas properties is that, despite their lower metallicities, high-z galaxies are often quite dusty (Scoville et al. 2016), requiring reddening corrections for widely separated lines.

JWST's NIRSpec will apply spatial and spectral resolution to z=2 similar to what e.g., SDSS's MaNGA (Bundy et al. 2015) reaches at z=0. Locally, resolved emission-line maps reveal metallicities and stellar surface mass densities correlate (Barrera-Ballesteros et al. 2017), with extra ionization and heating from AGN (e.g., Davies et al. 2017) or AGB stars (Yan & Blanton, 2012, Belfiore et al. 2016) towards the centers of galaxies, and shocks from winds (Rich et al. 2011). AGN and large-scale shocks can strongly bias unresolved galaxy metallicity measurements (Juneau et al. 2014). In the rare but informative cases where metallicity gradients have been measured at high-z, these galaxies have a more diverse set of metallicity gradients, often inverted (Jones et al. 2010). With *JWST*, we will finally *systematically* map high-z emission lines instead of just for rare systems. However, as AGN are both more common and more luminous, all of the complicating effects seen locally should be amplified at high-z (Newman et al. 2014).

4.3 The need for high circumgalactic resolution and a large suite of feedback models: The temperature, density, angular momentum, and metallicity of flows from the CGM can strongly affect interstellar gas (e.g., Sánchez-Almeida et al. 2014). As with the stellar distributions (§3), we found in our test cases that forcing refinement in the CGM has a profound impact on the *interstellar* gas. Physically, star formation and AGN feedback and winds will shock the gas and drive turbulence. How do the details of when, where, and how much heat and momentum is injected into the ISM affect emission line maps? With our large feedback parameter study, we will directly test how energy, momentum injection from all the sources affects star formation efficiency in z>2 galaxies.

4.4 It is only with synthetic observations based on realistically simulated galaxies that we can fully anticipate and interpret the upcoming wealth of observations from JWST: In aggregate, the above interstellar complications imply that while, e.g., directly measuring metallicity gradients from simulated galaxies can be informative, synthetic data are required for a complete picture of the *observable* physical conditions in z>2 interstellar gas. We will construct emission line maps and compare diagnostics to the underlying physical conditions the diagnostics are trying to measure (metallicity, temperature, shocks, etc.), at both the native resolution of the simulations and at the resolutions of relevant instruments, enabling us to test the efficacy and possible biases in various line ratio diagnostics. Our synthetic data will include the effects of dust attenuation, reddening, and scattering. In addition to the intrinsic bolometric AGN luminosity, we will also make predictions for the hard X-ray luminosity, which lacks significant contamination and acts as a direct measurement of SMBH accretion. Moreover, the FOGGIE simulations will enable test of AGN selection effects and diagnostic tools, such as spatially resolved line ratios (e.g., [OIII]/Hβ, Figure 3, Bridge et al. 2016) and line velocity profiles.

5. The circumgalactic medium: outflows, inflows, recycling, physical conditions

Deliverables: realistic mock spectra for Keck/HIRES, line flux and velocity measurements
Our Science: effects of feedback on the CGM properties and observables
Enabled Science: baryon budget evolution, galaxy/absorber statistics, large-scale structure, IGM enrichment, mock "down-the-barrel" spectroscopy of outflow and inflow, mock spectra for other instruments, emission-line maps, circumgalactic dust

We now have broad characterizations of the mass and metal content of circumgalactic gas and how it relates to galaxies. At low-z, the CGM mass equals or surpasses a galaxy's stars (Werk et al. 2014), encompassing a wide range of metallicities from 1% Solar to super-Solar (Lehner et al. 2013; Prochaska et al. 2017), but with kinematics consistent with being gravitationally bound to its galaxy. Star-forming galaxies appear to have more CGM gas when they have more ISM gas, suggesting a causal connection (Borthakur et al. 2014); yet quenched galaxies *also* retain a significant mass of cool CGM gas, apparently not accreting and using it to form stars (Thom et al. 2012). At $z>2$, the CGM appears in these same UV diagnostic lines shifted into the optical. The pioneering Keck Baryonic Structure Survey (Steidel et al. 2010; Rudie et al. 2015) combines Keck/LRIS spectra of galaxies with higher resolution (ESI or HIRES) QSO absorber data on about 300 galaxies. The inferred CGM masses are significant, but at $z>2$ it is more common to detect gas at high relative velocities, as if it is being ejected from its galaxy to the IGM (Turner et al. 2014). By contrast, there are few signs of accretion even at an epoch when galaxies *should* be fed more rapidly than they are today.

While simulations generally agree that the CGM harbors a significant fraction of the baryons that reside in dark matter halos, they disagree on both the details and the ionization states of this gas (Tumlinson, Peeples, & Werk 2017). The CGM harbors large amounts of cold gas ($T<10^4$ K) as far as 150 kpc from the centers of both passive and star forming galaxies (Thom et al. 2012), yet, likely owing to poor resolution, many simulations lack cool gas (Figure 1). Conversely, *Hubble* has found strong O VI (which is maximally abundant at $T\approx10^{5.5}$ K—curiously at the temperature where gas *should* cool most effectively) around star-forming galaxies with absorption profiles suggesting that gas in both phases are kinematically related (Werk et al. 2016). Yet different hydrodynamics solvers using a variety of feedback methods all have difficulties in reproducing the low and high ion data (Hummels et al. 2013, Liang et al. 2016, Oppenheimer et al. 2016, Suresh et al. 2017).

5.1 The gas-galaxy connection will get stronger at $z>2$: Three expected observational developments will greatly strengthen the observational CGM-galaxy connection in the next few years. First, the vast body of high-resolution spectroscopy with Keck's long-lived spectrographs is being published and analyzed by the KODIAQ survey (O'Meara et al. 2015; 2017), even while newer optical and IR instruments on 10-m class telescopes open up the frontier for $z>2$ CGM spectroscopy. Second, *JWST* galaxy redshift surveys in the fields of $z>4$ QSOs will associate galaxies with absorbers much further down the luminosity function than KBSS, encompassing dwarf populations, AGN, and galaxies on their way to becoming passive (e.g., GTO program LILLY_0001-0012). Third, emission-line mapping of circumgalactic gas with VLT/MUSE and Keck/KCWI is just beginning in earnest, providing constraints on gas density and extent that are complementary with absorption. These new observations create opportunity for theoretical insights and demand for synthetic data at a commensurate level of detail.

5.2 The power of "forced refinement": Data-derived estimates for the masses of "cool" clouds ($T=10^{4\text{-}5}$ K) range from $10^{4\text{-}6}$ $M_\odot$, comparable to *only one cell or particle in typical calculations* (Stocke et al. 2013, Faerman et al. 2016, McQuinn & Werk 2017). This temperature range may comprise a large fraction of all galactic baryons (Werk et al. 2014), but its major constitiuents *cannot* be resolved by conventional simulations. Furthermore, if the CGM is *not* resolved, then we cannot be sure that important global processes like accretion, feedback, and recyling are being followed correctly either. **Using forced refinement, we routinely reach mass resolution in the CGM that is 4–5 orders of magnitude better (smaller masses) than conventional calculations.** The effect of forced refinement on the evolution of the simulated CGM is shown in Figures 2 and 5. *Even with no changes to the underlying physical prescriptions*, resolution itself has profound affects on the physical structure and observed properties of the CGM: a richer, more variable density and temperature field develops, and we see more high-density/low temperature peaks than at lower resolution. These thermal flucucations can cool, collapse to dense clouds, and perhaps accrete into the galaxy. The effect is

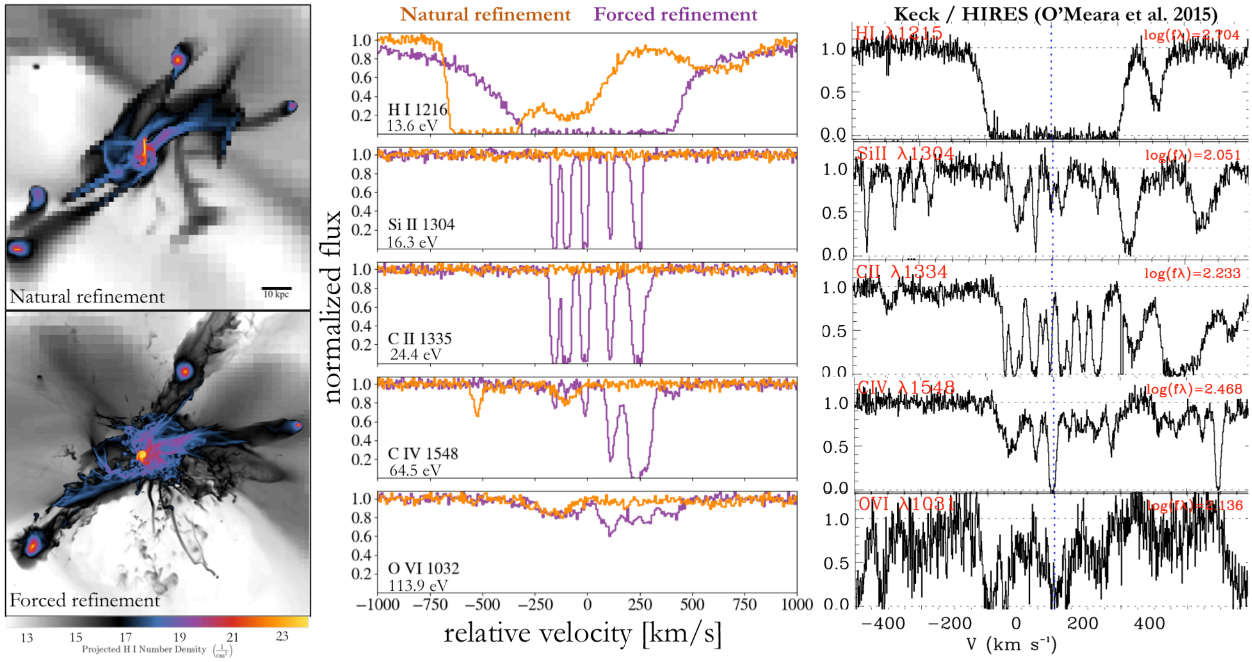

Figure 6: The simulated and observed CGM. *Left*: HI column density; Lyα is optically thick at about where the color is. *Middle*: synthetic CGM absorption lines at a range of ionization energies with the Keck/HIRES LSF and sampling, and a SNR of 30/pixel. *Right*: a typical (but relatively uncontaminated) real absorber CGM at z=2.13 from the Keck/HIRES KODIAQ survey; KODIAQ has several hundred such absorbers at z>2 (O'Meara et al. 2017).

also seen in the simulated spectra through a filament (Figure 6), which exhibits higher total column density and far more structure in the cold gas ions than the naturally refined run. The abundance of low-ion absorption produced with forced refinement (Figures 2 and 6) but not in the naturally-refined case is generic in our test cases over a wide range of redshift and physical inputs.

5.3 Subgrid physics via "flux tracking": Our approach for examining the mass, temperature, ionization, and metallicity distribution of the CGM is to compare it to how these quantities flow though its boundaries (in and out) instead of simply comparing to the values of the subgrid physical parameters. To do this, we define a boundary around the disk (~10 kpc above and below) and track the flux of mass, metals, entropy, and other key variables across this plane. The flows of mass and entropy that cross this plane are either inputs to the CGM (if they flow out from the disk), or arrive from the CGM (if the flow in). We can therefore track the properties of the CGM (its metal content, entropy profile, etc.) directly against the inputs. As we turn these knobs to increase or decrease the feedback, the CGM inputs crossing the flux-tracking boundary will change (but not necessarily linearly), as will the CGM properties. This method provides an insightful way of assessing physical correlations that is less sensitive to the exact details of feedback at the subgrid level, which are more difficult to compare across different prescriptions and simulation groups.

5.4 The need for synthetic circumgalactic data: It is only with synthetic spectra from cosmological hydrodynamic simulations that one can hope to disentangle the complexity inherent in real observed spectra arising from a multiphase dynamic medium (Figure 6). We need synthetic spectra to (1) fully understand the mappings between observable absorption components and physical "clouds", (2) disentangle the complex velocity profiles of multiple ions, (3) glean physical trends from observed lines for which columns cannot be measured (but velocity widths and equivalent widths can). For instance, when a single component is detected in observational data, we can quantify how "clouds" are blended together, along with their range of densities, temperatures, and abundances. These simulations will also enable mocking circumgalactic emission (Corlies & Schiminovich 2016).

5.5 The effects of star formation and AGN feedback on the CGM: Using the FOGGIE simulations, we will determine how star formation and AGN feedback affect the observable CGM at z>2. Simulations of the CGM to date have verified that feedback has a profound impact on the circumgalactic medium: it heats and enriches galaxies' gaseous halos, ejected material may recycle back into the ISM, and gas accreting into the halo may be prevented from accreting onto *galaxies* via interactions with outflowing material. With our feedback parameter study, combined with out flux tracking method and realistically mocked spectra, we will directly test how star formation and AGN feedback affect the ionization states, densities, temperatures, metallicities, *and* observable properties of circumgalactic gas. Moreover, by including self-consistent AGN, we will account for the effects that time-varying harder ionizing spectra have on non-equilibrium ionization and cooling that have been shown to strongly affect the low-z simulated CGM (Oppenheimer et al. 2017). Our high-resolution simulations are also optimized for following accretion from beyond R_{vir} all the way to the disk, determining how its trajectory depends on the galaxy's winds, and possibly deriving the observational signatures needed to find it.

6. Metals: Nature's tracer particles

Our Science: cosmic distribution of metals and metallicity scaling relations

Enabled Science: elemental abundance ratios in DLAs and old stellar populations at z=0, dust chemistry

6.1 Bringing it all together: Metals—*the unambiguous products of star formation*—provide a unique and natural tracer of the baryon cycle. As heavy elements are produced in stellar deaths, the buildup and initial distribution of the different elements is highly sensitive to galaxies' star formation histories (§3). Metals are most easily observed in the ISM (§4), where they trace flows of gas within galaxies. Large-scale winds driven by feedback expel the vast majority of metals into the CGM (§5). Thus chemical evolution neatly ties together the stars, ISM, and CGM comprising galactic ecosystems.

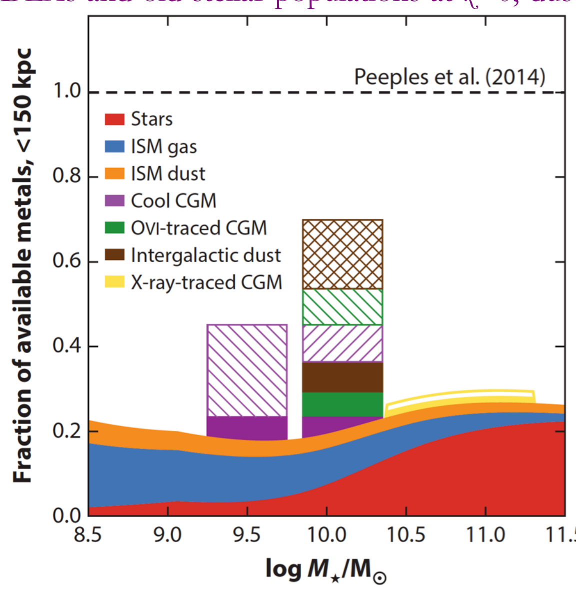

Figure 7: An accounting of metals in and around star-forming galaxies at z~0 from Tumlinson, Peeples, & Werk (2017).

6.2 A budget and accounting of galactic metals: By z~0, star-forming galaxies contain a surprisingly constant 20–25% of the metals they have ever produced in their stars, interstellar gas, and interstellar dust, with about the same metal mass found in the CGM out to 150 kpc (Peeples et al. 2014, see also Figure 7). The spatial extent and metallicity distribution of enriched gas are key constraints on feedback models that push metals out of galaxies. Simulations have long suggested (Oppenheimer & Davé 2006) that the CGM is enriched early (z>>4) by fast outflows that join the Hubble flow and re-accrete back onto halos at later times, though how consistent this picture is with the pockets of metal-poor dense gas observed at z>2 (§5) remains to be seen. *JWST* will revolutionize our ability to measure both interstellar gas *and* stellar abundances at z>2. The lever arm on cosmic time will help us understand how and when metals are deposited, how they relate to accretion, and how mixed the gas can be. While the z>2 CGM harbors a massive reservoir of baryons (Lehner et al. 2014), extremely metal-poor circumgalactic systems at z>2.5 (e.g., Fumagalli et al. 2011, Lehner et al. 2016) indicate that rare pockets of extremely low metallicity gas do exist. From Figure 2, it is evident that very low-metallicity gas can persist close to galaxies at these redshifts—at least when modeled with adequate resolution. We will track how the distribution of metals evolves in single halos, how it depends on the strength of feedback, and for how long the ISM and CGM metal patterns retain memory of disruptive events such as strong feedback episodes, AGN cycles, or mergers.

6.3 The origins of scaling relations: At all redshifts where it has been able to be measured, there is a tight relation between stellar mass and gas-phase metallicities (Tremonti et al. 2004, Erb et al. 2006, Mannucci et al. 2009). At z=0 there may (Mannucci et al. 2010, Andrews & Martini, 2013) be a secondary dependence on star formation rate, with higher SFR galaxies having lower gas-phase metallicities, though this signal is not found in samples spatially-resolved spectra (e.g., CALIFA, Sánchez et al. 2013 or MaNGA, Barrera-Ballesteros et al. 2017). Theoretically, however, a dependence of Z_{gas} on the star formation rate is intriguing, as the instantaneous SFR should correlate with galaxies' gas contents, which in turn dilute the available metals (Peeples et al. 2008, 2009, Peeples & Shankar 2011). Broadly, HI does provide a more robust third parameter than star formation rate (Bothwell et al. 2013, Jimmy et al. 2015), but interstellar HI is generally unobservable at z>0.3. Some observations have suggested that the Z_{gas}-$M_{\star}$-SFR relation does not evolve with redshift (e.g., Lara-Lopez et al. 2010), which can be understood from a gas regulation model (Davé et al. 2012, Lilly et al. 2013), with feedback-driven outflows modulating the overall metallicity level and its dependence on stellar mass. However, whether or not such a relation, if it even exists at z=0, does not evolve with redshift remains controversial in the literature (e.g., de los Reyes et al. 2015). The time evolution of individual galaxies is key to disentangling the competing effects of more gas diluting the ISM's metals (leading to lower metallicities), but more gas leading to more star formation (and thus more metal production and higher metallicities). In particular, with FOGGIE's synthetic data we will be able to quantify the lags between the (unobservable) changes in HI and tracers of star formation, such as Hα emission. Moreover, observed high-z galaxies have a broader diversity of metallicity gradients than the local galaxies: understanding the spatial distribution of metals *within* galaxies will be even more important at z>2.

6.4 The role of FOGGIE: We will address the observability of each of these metal phases: stars, interstellar gas *and dust*, and the CGM. Part of the exquisite power of using metals as tracer particles is the different elemental cocktails arising from core-collapse supernovae, Type Ia supernovae, and AGB stars. By tracking different elements, FOGGIE will trace how elements produced in varying locations at different times are transported within and out of galaxies—and how these differences depend on the strength of feedback. Adequately resolving the CGM is critical to tracing metals: metal-rich gas cools more effectively than metal-poor gas, and so if the CGM is unnaturally well-mixed owing to coarse resolution, then the metallicity of accreting and recycling gas may also be inaccurate. Our feedback study combined with our flux tracking scheme will also give us new insights into how metals cycle: intuitively, the redistribution of metals *should* be highly sensitive to the strength of galaxy outflows. Furthermore, we will use *actual* simulated tracer particles for short periods of cosmic time to, e.g., explicitly track there where the metals produced by individual bursts of star formation and the origin and fate of circumgalactic (e.g., Ford et al. 2014).

7. Concluding Thoughts and Proposed Timeline

The FOGGIE simulations and associated synthetic data will address important open questions regarding how gas flows in, and between, the CGM and ISM connect to resolved interstellar gas and star formation histories at z>2. By pursuing these questions as one group and in parallel (see Table), our picture of the gas-galaxy connection will be fuller than if this work was done independently.

Management structure, work breakdown, and proposed timeline				
Person	**Preparation**	**Year 1**	**Year 2**	**Year 3**
Molly Peeples (PI)	MISTY code devel (§2.4), IC selection	Run sims, code devel, train postdocs	Author MISTY-CGM paper, run sims, co-author papers	Run sims, co-author papers
Jennifer Lotz (Co-I)	IC selection	MISTY code devel.	Co-author papers	Co-author papers
Gregory Snyder (Co-I)	MISTY code devel, IC selection	Train postdocs, code devel	Author MISTY-galaxies paper, co-author papers	Co-author papers
Jason Tumlinson (Co-I)	Code devel, IC selection	Run sims, train postdocs	Co-author papers	Run sims, co-author papers
Postdoc #1 CGM & Metals Specialist	. . .	Run sims, MISTY & analysis code devel.	Author CGM & metals papers (§§5,6)	Other projects + co-author papers
Postdoc #2 Morphology & ISM Specialist	. . .	Other projects + run sims	Run sims, Enzo code devel., co-author papers	Author ISM & stars papers (§§3,4)
Brian O'Shea (Institutional PI)	Enzo code devel (§2.3), IC selection	Code devel., run sims	Code devel., run sims	Run sims, co-author papers
Lauren Corlies (Collaborator)	Code devel	Help train postdocs	Co-author papers	Co-author papers
Britton Smith (Collaborator)	Generate ICs	Code devel. (Grackle)	Co-author papers	Co-author papers
Undergraduates (MSU & STScI)	…	Visualizations & test MISTY code	Visualizations & test code	Visualizations

8. You might be wondering…

Why two postdocs instead of one, or a graduate student? Two concurrent postdocs will be more productive than one with a longer appointment. Learning both numerical hydrodynamics *and* observational effects is too much to expect of a graduate student; critical to this program's success is that the postdocs are trained to learn the relevant observational and instrumental complications.

Why Enzo? Why not use a simulation code that has already "calibrated" its feedback prescriptions? No existing simulations adequately resolve to the CGM. Grid codes are best for high resolution in low-density gas and only Enzo already has enough physics in it (including sophisticated hearting/cooling, star formation, etc.). We have already implemented forced refinement and flux tracking for our low-z CGM research. Once we have implemented some new feedback, Enzo will be at the state of the art for galaxy formation simulations.

The scope of this work seems too ambitious for the funding requested. In addition to the funded effort, the four STScI co-I's all have twelve month salaries and are prepared to commit a cumulative three years worth of effort to this project should it be funded. Peeples, O'Shea, Tumlinson, Lotz, and Snyder all have experience with simulation projects at this scale and regard the plan as feasible.

What is this awesome font you're using? Thank you! It's called Garamond, and we love it because the z is super-cool looking!

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