

Figuring Out Gas & Galaxies in Enzo (FOGGIE): Mapping the Baryon and Metal Cycles

1. Target problem: the role of diffuse gas in evolving galaxies	2
1.1 <i>The observational and simulated landscape</i>	2
1.2 <i>Suitability for NASA's ATP</i>	2
1.3 <i>How to read this proposal</i>	3
2. A new suite of cosmological hydrodynamic simulations: FOGGIE at the Exascale	3
2.1 <i>ENZO-E + overall scheme</i>	3
2.2 <i>Starting strong: unprecedented intergalactic resolution in FOGGIE:R</i>	5
2.3 <i>Exploring physics and numerics in cosmological subvolumes</i>	5
2.4 <i>Bringing it all together: the FOGGIE:ST simulation</i>	7
3. A close connection to observations and the role of synthetic data	8
4. Flux tracking: a new approach to connecting the CGM and galaxy evolution	9
5. Galaxy scaling relations and the evolving baryon census	11
6. The evolving metal census and global circumgalactic statistics	12
6.1 <i>Metals: Nature's tracer particles</i>	12
6.2 <i>The evolving circumgalactic distribution of metals</i>	13
7. Angular momentum exchange and the evolution of galaxy morphologies	13
7.1 <i>The observed kinematic and morphological evolution of galaxies</i>	13
7.2 <i>Circumgalactic gas exchanges angular momentum with galaxies</i>	13
7.3 <i>Angular momentum tracking and observing morphological evolution</i>	14
8. Concluding thoughts, team management, and proposed timeline	15
8.1 <i>The FOGGIE collaboration</i>	15
8.2 <i>This grant's timeline</i>	15
9. You might be wondering...	16
References	17
Biographical Sketches	22
Table of Work Effort	29
Current and Pending Support	30
Budget Narratives	39
Budgets	44

Figuring Out Gas & Galaxies in Enzo (FOGGIE): Mapping the Baryon and Metal Cycles

We request 3 years of funding, primarily to fund a postdoc and a graduate student, to address how galaxy populations evolve by providing a major step forward in our ability to analyze the connection between galaxies and their circumgalactic gas. We propose (1) to run and analyze a suite of cosmological domain simulations with unprecedented IGM and CGM resolution, (2) to interpret the evolution of the galactic scaling relations, the redistribution of metals, and the evolution of galactic kinematics based on the physical fluxes in and out of galaxies and the CGM, and (3) to generate and make publicly available synthetic data based on these simulations for connecting these physical properties directly to the observables.

1. Target problem: the role of diffuse gas in evolving galaxy populations

1.1 The observational and simulated landscape: Galaxies evolve by accreting gas from the diffuse intergalactic medium (IGM) and converting that gas into stars. Those stars then energetically expel freshly created heavy elements back into the cosmic web; this star formation feedback in turn drastically alters the gas around the galaxy, known as the circumgalactic medium (CGM), where it is sometimes recycled into accreting fuel for galaxies at later times. The detailed physics of how these baryon and metal cycles vary across time and halo mass underlies the observed scaling relations between galaxy mass, star formation rate, metallicity, size, morphology, etc., at all epochs. This theoretical picture has begun to be revealed in the low-density gas itself, with observations showing that some—but not all—physical properties of the CGM depend on galaxy mass (Werk et al. 2014; Johnson et al. 2017; Bordoloi et al. 2018), star formation rate (Tumlinson et al. 2011; Borthakur et al. 2016; Zahedy et al. 2019), environment (Burchett et al. 2016), and redshift (Chen et al. 2017). In tandem, cosmological hydrodynamic simulations have had increasing success at producing realistic galaxies (Christensen et al. 2010, Somerville & Davé 2015, Hopkins et al. 2018), but generically struggle to do so while also producing gaseous halos with observed properties (Tumlinson, Peeples, & Werk 2017). Recently, several groups, including our own, have shown that part of the problem is that the simulated CGM is chronically under-resolved (Peeples et al., 2019 [hereafter, FOGGIE I]; Corlies et al., 2019 [hereafter, FOGGIE II]; van de Voort et al., 2019; Suresh et al., 2019; Hummels et al., 2019; Rhodin et al. 2019).

Meanwhile, observations continue pushing towards understanding galaxies and the CGM *together*, which demands a response from theory. To be effective, simulations must statistically sample galaxies in a range of environments and states of evolution while *also* resolving the low-density gas pervading the cosmic web and the circumgalactic medium. **We propose here to run and analyze new cosmological domain simulations aimed at exploring the co-evolution of galaxies and the CGM with unprecedented resolution of the low-density gas driving galaxy evolution.** These simulations will provide a crucial first step towards realizing these goals and will enable new and unique insights into interpreting observations of the co-evolution of gas and galaxies.

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 Keck, *Hubble*, *JWST*, and *WFIRST*. Our broad program surpasses the scope and funding scale of the *Hubble* theory program. With *JWST* set to be launched in Spring 2021 (before the next ATP deadline), it is important that we begin this work *now*.

1.3 How to read this proposal: We propose here to run and analyze a new suite of cosmological domain simulations with unprecedented intergalactic and circumgalactic resolution aimed at understanding how the fluxes between galaxies and the CGM affect their co-evolution. We describe our proposed simulations in §2, the role of synthetic data in §3, and our novel “flux tracking” approach to simulation

analysis in §4. Our broad science goals are to understand the evolution of galactic and circumgalactic baryons (§5), the buildup and redistribution of metals (§6), and the exchange of angular momentum between galaxies and the CGM (§7). We conclude with our team management structure, proposed timeline, and final thoughts in §§8 and 9.

2. A new suite of cosmological hydrodynamic simulations: FOGGIE at the Exascale

We describe here our simulation code ENZO-E and our proposed simulation scheme in §2.1, which involves the FOGGIE: Round-1 (FOGGIE:R) simulation to be run in Year 1 (§2.2), a parameter-space study using a suite of smaller subvolumes (§2.3), and the FOGGIE: Second Try (FOGGIE:ST) simulation (§2.4) to be run in Year 3.

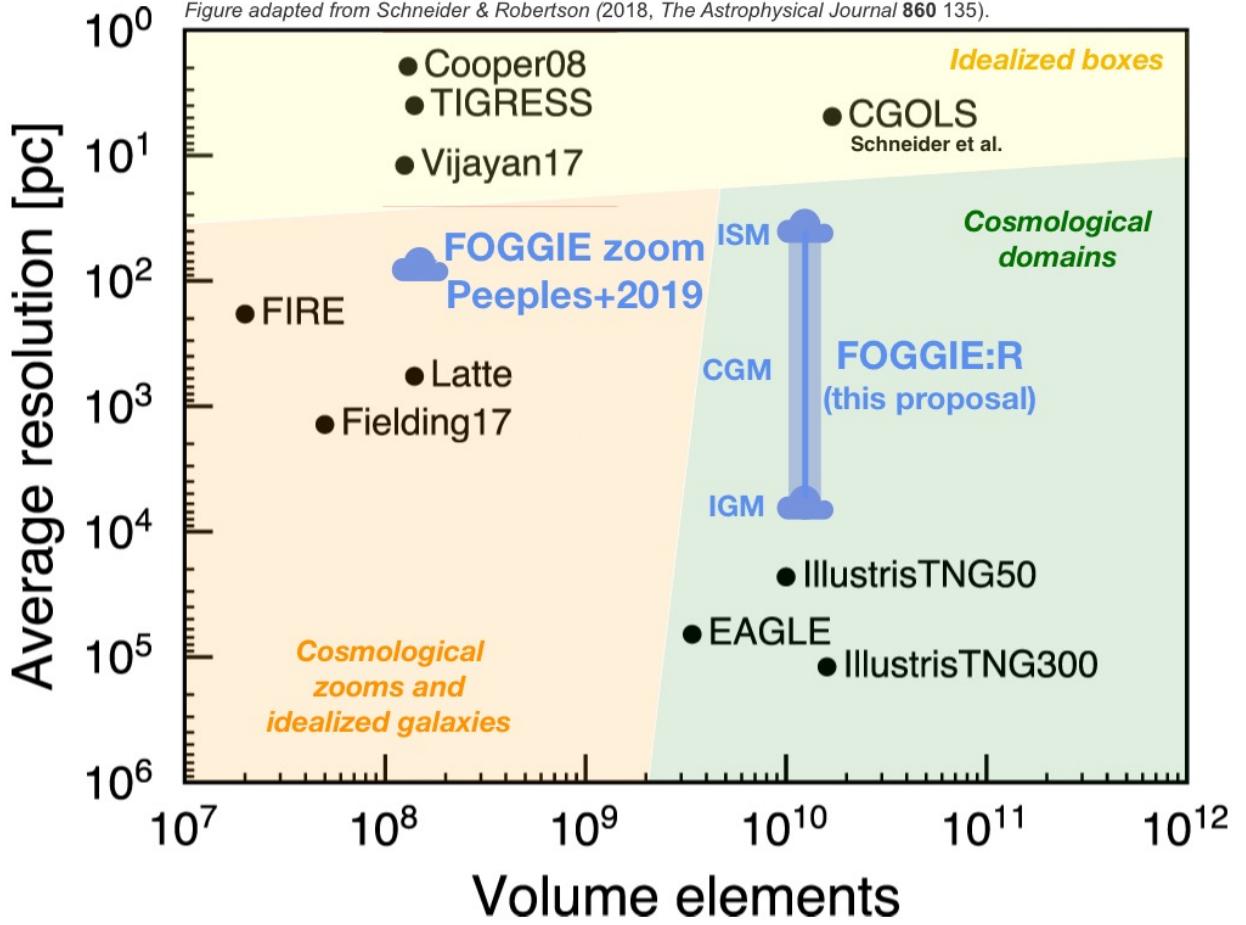


Figure 1. The existing and proposed FOGGIE simulations in context of existing hydrodynamic simulations aimed at understanding galaxy evolution (adapted from Schneider & Robertson 2018). Our long-term goal is to achieve the spatial (and mass) resolution in the current FOGGIE zooms over an entire cosmological domain; our FOGGIE:R simulation will be an important first step towards realizing this goal. What we will learn from our smaller subvolume simulations will help us push the FOGGIE:ST simulation to better spatial resolution (and subgrid physics modules) while efficiently making use of available computing resources.

2.1 ENZO-E + overall scheme: We will use the ENZO-E code to evolve a cosmological volume of $(25 \text{ cMpc}/h)^3$ to $z = 0$. ENZO-E (Bordner & Norman 2012, 2018) is a complete redesign of the original Enzo code (Bryan et al. 2014) for the exascale era and is built using the Charm++ parallel

programming system, which has a data-driven, asynchronous execution model (<http://charm.cs.uiuc.edu/>). ENZO-E implements its adaptive mesh refinement algorithm using a fully distributed “forest of oct-trees” data structure and has a new, highly scalable gravity solver. All of the physics modules from the original ENZO code, including microphysics such as cooling, chemistry, and metagalactic UV backgrounds, star formation and feedback algorithms, supermassive black hole formation and feedback algorithms, (magneto)hydrodynamics, and radiation transport, are being ported to ENZO-E. While being ported, they are being converted from Fortran or C to C++ so that the code will be performance-portable using the Kokkos framework (<https://github.com/kokkos/kokkos>). This will allow ENZO-E to run on both CPUs and GPUs, which is particularly important because future generations of supercomputers will be dominated by GPU-like architectures. Taken together, **ENZO-E represents a highly flexible, performant, and scalable platform for the study of cosmological structure formation in the exascale era**. ENZO-E’s development has been ongoing for several years, and is currently heavily supported by large, multi-institution NSF grant ([OAC #1835402](#)) that ensures a rapid growth in ENZO-E’s capabilities and substantial community support in the future. Using ENZO-E, we will be able to perform cosmological calculations that are *orders of magnitude* larger than the current state-of-the art, and which are effectively limited only by (1) the amount of memory on a given supercomputer and (2) the amount of computing time available for the calculations. Combined with ENZO-E’s low memory footprint, these advances will enable us to reach unexplored regions of simulation parameter space (see Figure 1).

Our simulation strategy is to bracket the duration of this grant with two large ($[25 \text{ cMpc}/h]^3$) refine-everywhere simulations to explore the behavior of large populations of galaxies over a range of masses and environments, with a suite of smaller, shorter duration, and faster simulations for testing and parameter space exploration in the interim. At $\zeta=2$ there will be a $\sim 2,400$ halos with virial masses above $10^{10} M_\odot$, ~ 240 halos above $10^{11} M_\odot$, and ~ 17 above $10^{12} M_\odot$. This volume will thus contain large numbers of galaxies in significantly under- and over-dense environments, enabling us to explore how the galaxy-CGM connection depends on both mass *and* environment.

We will generate all of these initial conditions using the same initial seed as our pilot simulation¹ (from which we are selecting halos for zooms as part of a previously-funded research program), which had a 512^3 root grid and 6 levels of refinement² (i.e., the same ISM resolution as the FOGGIE:R simulation will have, but an $4\times$ coarser intergalactic resolution; see Figure 2). By using the same seed as for our zoom simulations, we will additionally be able to investigate the effects of the updated numerics and physics on the evolution of these ~ 25 halos with even more detail.

Most, if not all, published cosmological domain simulations aimed at understanding galaxy evolution are at fixed mass resolution—which places a fundamental limit on how *spatially* well-resolved the low-density gas in these simulations is (see FOGGIE I). Though the ISM resolution and feedback models we propose here are perhaps not “groundbreaking” with respect to more established codes, improving the spatial resolution *in the vast majority of the cosmic volume* will provide an important step towards fully modeling how galaxies evolve in the cosmic web. Conversely, our base level improvement of $4\times$ better spatial IGM resolution translates to an improvement of $64\times$ *mass* resolution at fixed density—and as we have found in the FOGGIE zooms, improved spatial resolution allows previously uniform gas to form substructures, leading to a wider range in the masses of individual resolution elements (i.e., cells).

¹ This pilot simulation only has thermal feedback from supernovae and does not have self-shielding implemented, making it unfeasible to use to predict what we will find with FOGGIE:R’s more complete physics modules.

² The spatial scale per cell decreases by a factor of two for every increase in refinement level.

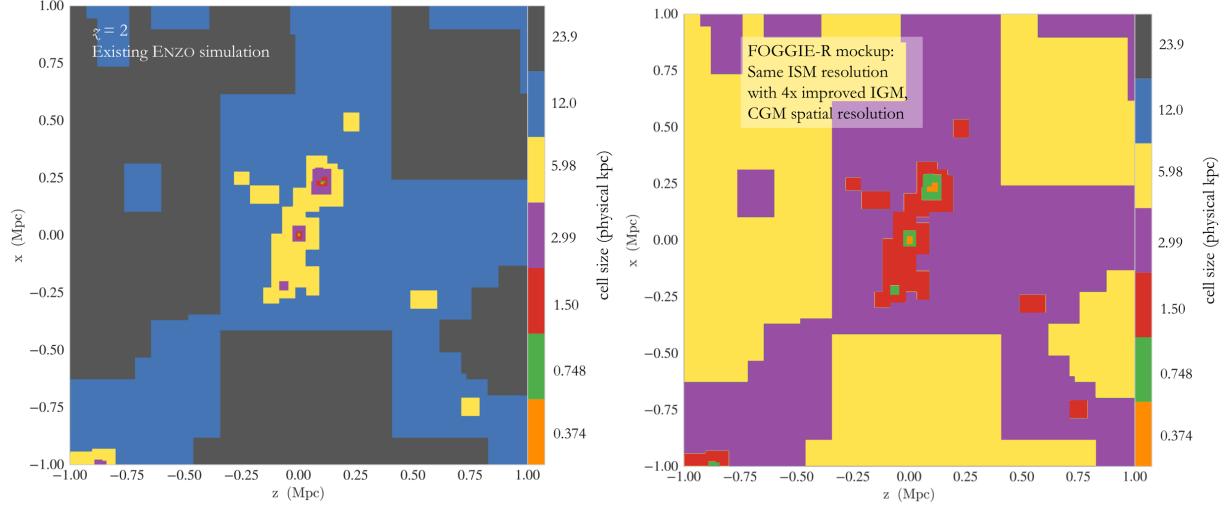


Figure 2. A slice through the densest region of a pilot ENZO simulation, showing the resolution (in physical units at $z=2$) in this simulation (*left*) and in a mockup of proposed FOGGIE:R (*right*). The standard-resolution simulation has a root grid of $(2^9)^3 = 512^3$ cells and $n_{\text{ref},\text{max}}=6$ levels of refinement, while FOGGIE:R will have a root grid of $(2^{11})^3 = 2048^3$ and $n_{\text{ref},\text{max}}=4$, reaching the same resolution of the dense gas while natively resolving the tenuous IGM and CGM at a $4\times$ smaller finer spatial scale. While the resolution typically quoted for cosmological simulations is that of the smallest scales resolved (i.e., in the ISM), the *vast* majority of the volume is often modeled at spatial scales one to two *orders of magnitude* coarser than the ISM. Though ENZO is unable to efficiently scale to the size of FOGGIE:R, this is exactly the kind of calculation ENZO-E is designed for.

2.2 Starting strong: unprecedented intergalactic resolution in FOGGIE:R: For the first bracketing simulation, FOGGIE: Round-1 (FOGGIE:R), **we will use a root grid of 2048^3 , giving a coarsest resolution of $12.2 \text{ ckpc}/h$ everywhere**, with 4 levels of refinement, yielding sub-kpc resolution (763 cpc/h) in the interstellar medium (see Figure 2). We will use our current cutting-edge physics models, including primordial gas chemistry and metallicity-dependent cooling using the Grackle library (Smith et al. 2017), both of which will include self-shielding, a grid-based implementation of the FIRE-2 star formation and feedback algorithm (Hopkins et al. 2018), and AGN feedback using a modified version of the Meece et al. (2017) model. We have these initial conditions in hand and will be able to start running the simulation immediately upon award of the associated computing time (April 2020, about six months before the STScI postdoc would start). Moreover, **our finer root grid will yield dark matter particle masses of $115,000 M_\odot$** and minimum star particle masses of $6,250 M_\odot$, allowing us to resolve smaller galaxies than in many other cosmological hydrodynamic simulations, e.g., the IllustrisTNG50 (100) simulation has dark matter particle masses of 4.5×10^5 (7.5×10^6) M_\odot , albeit in larger volumes (Pillepich et al. 2018). This first calculation will have current-generation physics and exceptional spatial and mass resolution, giving us the best-ever view of the evolution of the CGM and IGM while still also providing resolution within galaxies that is competitive with current cutting-edge cosmological calculations (Figure 1).

2.3 Exploring physics and numerics in cosmological subvolumes: During the first two years of this grant, we will generate sets of initial conditions that focus our computational efforts on relatively small ($\sim [5 \text{ cMpc}/h]^3$ in size) subvolumes of the FOGGIE:R run. These initial conditions will have the same mass and spatial resolution in the volume of interest as the earlier run, but constraining refinement to a small subvolume will greatly reduce the overall computational cost, **enabling us to explore a broad range of physical and numerical parameter space**. All of the code developed as part of the

simulation campaign described above will be provided back to the ENZO-E community, as we have done and are continuing to do for our improvements to the original ENZO code. With respect to the underlying physical prescriptions, we will explore:

1. Varying star formation and feedback prescriptions from our current FIRE2-like prescription (Hopkins et al. 2018), and also varying our supermassive black hole feedback prescriptions (e.g., Meece et al. 2017), to explore the impact that these varied prescriptions will have on CGM observables. Given that these prescriptions are phenomenological approaches to modeling the behavior of stellar and compact object populations (see §4), this represents a baseline for uncertainties in our predictions as well as an opportunity to explore new prescriptions that are tuned for the strengths of mesh-based codes.
2. Varying our prescriptions for supermassive black hole seeding (i.e., the placement of relatively low-mass SMBHs in galaxies at high redshifts, as a phenomenological treatment of feedback missing from large-volume cosmological simulations) and growth. Toward this end, we will develop an in-line halo finder in ENZO-E, enabling us to vary prescriptions for, and gauge the impacts of, black hole injection and growth (and to compare to similar prescriptions in the Romulus and Illustris TNG projects; Tremmel et al. 2017, Pillepich et al. 2018).
3. Varying the included physics, including the shape and evolution of the metagalactic UV background, the properties of cosmic ray physics (e.g., the impact of cosmic ray diffusion vs. streaming; Butsky & Quinn 2018), and the properties of plasma physics (magnetic fields, thermal conduction, viscosity; Hopkins et al. 2019) on circumgalactic observables.

With respect to the numerics, “convergence” is challenging to define in multi-physics simulations because the different pieces of physics have different dependence on spatial and mass resolution (e.g., hydrodynamics vs. chemistry vs. stellar feedback). As a result, the meaning of a “resolution study” in this context is difficult to precisely determine, and thus to quantify. Rather than choosing our simulation parameters based on an ill-posed convergence criteria, we determine spatial and mass resolutions that physical arguments (e.g., the cooling length; Figure 2) suggest will resolve the phenomena we wish to study, and match our subgrid models for star formation, feedback, and AGN formation and feedback to those parameters—while optimizing the tradeoff between resolution and computing efficiency. With these ideas in mind, we will explore:

1. Doing simulations with $2\times$ ($8\times$) and $1/2$ ($1/8$) fundamental spatial (dark matter and baryon mass) resolution but with the same standard physics. These tests will allow us to push further down the mass function in addition to providing baselines for the computational expense of adding resolution everywhere and tests for how simulation resolution affects galactic and circumgalactic observables.
2. Varying the refinement techniques used: allowing refinement based on ensuring that the “cooling length” is resolved everywhere in the refinement volume (see Figure 3), and separately having very aggressive refinement criteria based on matter overdensity. This will explore the impact of our choice of refinement criteria on IGM and CGM observables. Our preliminary tests in the zooms show that a hybrid cooling+overdensity refinement scheme may be a more efficient use of computing resources than refining on overdensity alone.
3. Including tracer particles to follow the flow of baryons using a Lagrangian technique. This will allow us to directly measure the motion of gas in our simulations, and be used to calibrate our flux tracking tools (which will be used to analyze all of the simulations; §4). ENZO-E does not currently have tracer particles implemented, but the code has infrastructure for an arbitrary number of particle types and it is straightforward to port ENZO’s tracer particle methods into ENZO-E.

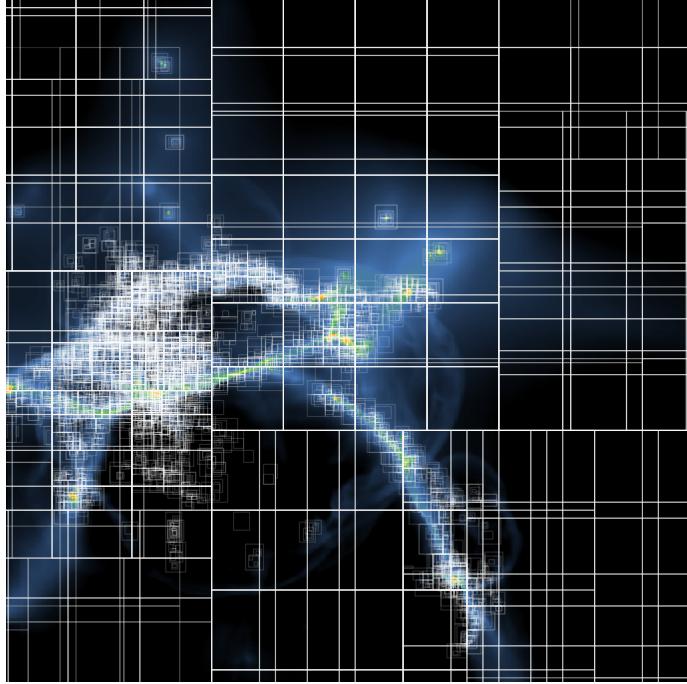


Figure 3. A projection of gas density at $z=4$ showing how our new “cooling refinement” works from one of our zoom simulations within a $(150\text{kpc})^3$ region. The white lines denote where the ENZO grids are. Instead of adding refinement to just the dense gas, we also refine based on the local cooling length (i.e., the product of the cooling time and the sound speed), as this is a critical physical scale that is generally not resolved in the IGM and CGM of cosmological simulations. Cooling refinement directly leads to improved spatial resolution along cosmic filaments, as can be seen by eye with more grids along the filament in, e.g., the bottom center. We will explore schemes for using cooling refinement over the entire cosmological domain as a way to improve IGM resolution in a computationally efficient manner.

More broadly, we will examine quantities that are robust to our numerical assumptions. [Genel et al. 2019](#) demonstrate that small changes in initial conditions for a single galaxy can result in changes in quantities such as star formation history at the level of 20–25%, with the differences primarily resulting from the chaotic interactions from feedback from subgrid feedback; our own tests with the FOGGIE zooms are consistent with this finding. Genel et al. find this “butterfly effect” does not substantially change galaxy scaling relations, but *does* contribute to their scatter (and is also seen in earlier studies using simpler simulations; e.g., Kandrup et al. 1994, Thiébaut et al. 2008, Sellwood & Debattista [2009](#), Boekholt & Portegies Zwart [2015](#)). The implication for our work is that, while individual absorbers from a particular species or galaxy morphologies may be impossible to compare between simulations, aggregate quantities (e.g., column density distributions for species in the CGM, or the relationship between bulk CGM properties and the star formation and feedback and/or AGN feedback histories of galaxies) *will* be robust to this type of stochastic behavior. This kind of comparison is also possible in simulations focusing on single galaxies (e.g., our zoom simulations), but comparisons between simulations of this type with different physical prescriptions, resolution, etc. will have to be interpreted carefully and concentrate on aggregate (and possibly time-averaged) quantities.

2.4 Bringing it all together: the FOGGIE:ST simulation: These tests will help inform which combination of methods is the most efficient and scientifically interesting for our second large refine-everywhere simulation, FOGGIE: Second Try (FOGGIE:ST). **This FOGGIE:ST simulation will have both improved physics modules and better resolution** informed by the suite of smaller simulations, and thus should be a better representation of the physical processes that are at work in galaxy evolution. Because we will have already developed our analysis tools, we will be able to analyze this simulation as it evolves (and thus before the end of this grant period). Therefore, while we frame the science goals of this proposal in terms of the FOGGIE:R and subvolume simulations parameter space search, we expect these same analyses to be applicable to the FOGGIE:ST simulation as it becomes available and for these results to be included in at least some of the Year 3 papers.

3. A close connection to observations and the role of synthetic data

A key piece of the FOGGIE program is a close connection to observational data. We will construct synthetic data of both circumgalactic absorption and of galaxy structural parameters in imaging and doppler spectroscopy. Our team has expertise in generating concrete observational comparisons from cosmological simulations, using an array of tools developed previously for the FOGGIE zooms and other simulations (FOGGIE I & II; Simons et al. 2019; Snyder et al. 2011, 2019). For this program, we will focus these efforts on measuring gas and stellar angular momenta and morphologies and circumgalactic absorption spectroscopy. **These synthetic data will be released publicly as we have done and are doing for the FOGGIE zooms.** We generate synthetic circumgalactic absorption spectra using our modified version of the Trident code (Hummels, Silvia, and Smith 2017), as done in the FOGGIE I paper, and our automated spectral analysis software SPECTACLE (Earl & Peebles, in preparation; <https://spectacle-py.readthedocs.io>). These spectra will be aimed at Keck/HIRES, Keck/LRIS, and Keck/KCWI for the high- z CGM and *Hubble*/COS and *Hubble*/STIS for the low- z CGM. For the synthetic galaxy data, we will adapt the tools that our team is developing via separately funded efforts for the FOGGIE zooms. We will focus primarily on imaging (see Figure 3), supplementing with H α spectroscopy to trace the kinematics as done in, e.g., Simons et al. (2019).

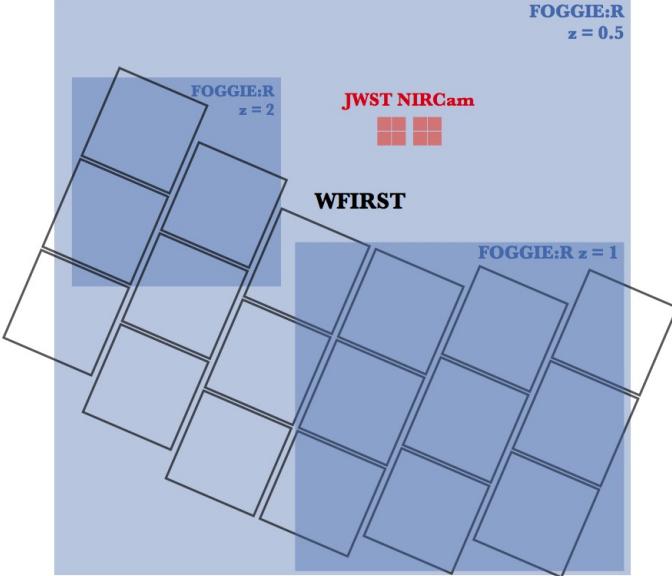


Figure 4. Simulating populations of galaxies large enough to compare to state-of-the-art datasets requires much larger volumes than in individual halo zoom simulations. FOGGIE:R’s cosmological volume is comparable to the size of the *WFIRST* field-of-view for imaging and grism spectroscopy, placing it in the first generation of simulations that covers large samples of galaxies while *also* optimizing for galaxy gas flows.

Our team is heavily involved with several past, ongoing, and future NASA-supported observational programs (e.g., COS-Halos, KODIAQ, and CEERS) with direct relevance to the science aims of this proposal. Of specific interest, the Keck Online Database of Ionized Absorbers towards Quasars (KODIAQ) is a long-term ongoing effort to mine the Keck Online Archive for $z \geq 2$ circumgalactic absorbers and associated galaxies. The grant that initially supported FOGGIE (NSF AAG #1517908; also led by this PI) supported the release of KODIAQ DR2 (~ 300 quasars; O’Meara et al. 2017) and will support the release of KODIAQ DR3 (the ESI data; O’Meara et al., 2019, in preparation). Furthermore, over the duration of the grant proposed here, it will support the data release of galaxies associated with the KODIAQ circumgalactic absorbers as observed with Keck/LRIS and Keck/MOSFIRE. (DR1 was supported by NASA via ADAP-NNX10AE84G; O’Meara et al. 2015.) While the FOGGIE zooms we are currently running and analyzing will go a long way towards helping interpret the detailed kinematic profiles of these CGM absorbers, we will need cosmological domain simulations like the ones we propose here in order to understand these data as a whole. While the KODIAQ program is the one we are most closely involved with (e.g., the FOGGIE I paper included

a fresh analysis of KODIAQ Lyman-limit systems), *JWST* will be used to obtain new views of galaxies in the fields of high- ζ quasars (e.g., GTO program [LILY 0001-0012](#)). The synthetic data we will make publicly available from our proposed simulations will help interpret these data and plan observational proposals for similar observations. For our purposes, by analyzing galaxy populations in *observable* space (especially for the subvolume experiments), we will be better informed when choosing with which physical parameters to run the FOGGIE:ST simulation, and in subsequently understanding their impact on the observable universe.

4. Flux tracking: a new approach to connecting the CGM and galaxy evolution

Our ultimate goal is to understand the physical processes that drive galaxy evolution, and how these vary with galaxy mass and time to give rise to the diverse populations we see in the real universe. Every attempt to do this in simulations *must* eventually come to grips with “subgrid” physical prescriptions. FOGGIE is no exception, but we do employ a novel approach to interpreting our results that reduces the role of the exact details of the subgrid physics, with beneficial effects on our interpretations with respect to data.

To create realistic galaxies, hydrodynamic simulations must include physical effects, such as supernova and AGN feedback, that deposit thermal and kinetic energy, heavy elements, cosmic rays, and dust back into their environments and which can affect a galaxy’s global evolution when they act and interact on galactic (kiloparsec) scales. Yet, all these phenomena arise on much smaller scales—from individual stars, clusters, or AGN that occupy parsec scales, or smaller. To make progress, simulations must contain instructions for how to, e.g. convert mass in a cell into a star particle, or how to deposit thermal and kinetic energy from the star particle back into the adjoining cells. We use the word “instruction” here deliberately to convey that these rules abstract away physical equations in favor of simple prescriptions; supernova feedback might be, for example, “when the star particle reaches 2 *million years* since its creation, add 10^{52} *erg* to the local thermal energy field and impart the surrounding cells with 100 km s^{-1} worth of kinetic energy moving away from the particle.” When stated this way, it becomes clear that the “feedback instructions” are governed by abstract parameters (italicized here). Different simulation codes and groups treat these parameters differently. They might fix some and vary others to achieve an optimum fit to observables such as the galactic stellar mass function or mass metallicity relation. They might pin some parameters down to either observations or simulations obtained at smaller physical scales and then hold them fixed throughout the runtime of the simulation, or let them vary somehow with redshift and/or galaxy mass.

The key point is that once these subgrid parameterizations have done what they do—create stars and drive feedback—the details of their instructions are not comparable from simulation to simulation, and neither are they able to support analysis of *observable* outcomes in terms of *physical* inputs. If we have obtained a galaxy mass function, or mass-metallicity relation, from a simulated galaxy population, how can we interpret its similarity to real data in terms of the three italicized parameters above? How can we compare our simulation results to others who write their instructions differently?

The way to cut this knot is to shift the basis for comparison to physical inputs. We call this approach “flux tracking.” Rather than basing comparisons on the details of the subgrid instructions, we define a boundary around the galaxy and track the flux of mass, metals, entropy, and other key variables across this surface. (We also define multiple shells and non-spherical shells when a more fine-grained approach is desired.) The flows of mass and entropy that cross this surface are either inputs to the CGM (if they flow out from the disk), or arrive from the CGM (if they 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, as will the CGM properties (with the change not necessarily being

linear). 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. By adding tracer particles to ENZO-E and running tests in our subvolume simulations, we will calibrate the “true” fluxes against the net fluxes that flux tracking captures in a more scalable fashion. This will also enable us to make more direct comparisons to previous results based on Lagrangian codes that connect the origin and fate of circumgalactic gas with observable ions of interest (e.g., Ford et al., 2014, 2016) and higher-resolution idealized simulations of the CGM (e.g., Fielding et al., 2017).

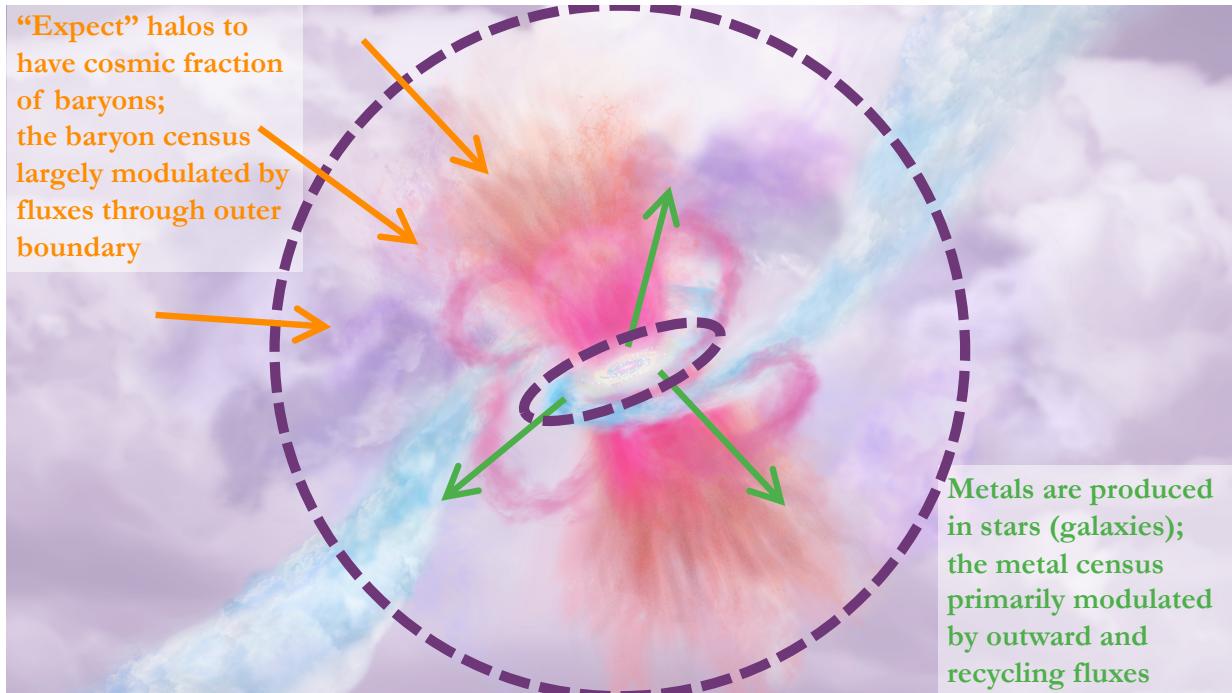


Figure 5. Our group has developed a scheme for tracking physical fluxes across boundaries that we call “flux tracking.” We track, e.g. energy, temperature, mass, metals, entropy, etc. over time at the virial radius, to and from the disk, and through annuli between these “boundaries.” Following these fluxes as the independent causal variable is superior to using the more arbitrary parameters from the subgrid physical prescriptions, which usually have the same values for all galaxies at all times. Flux tracking provides an explanatory power for galaxy scaling relations that otherwise does not exist. (Figure adapted from Tumlinson, Peeples, & Werk 2017).

Flux tracking takes on a much greater importance when we aim to simulate galaxy populations across a wide range of mass, as we do here. In this case, the **galaxy-wide outcomes are in fact emergent properties from a highly complex interaction of all the subgrid prescriptions**, which generally are not written down as a function of galaxy mass. If the parameters do not change with mass, but the outcomes do, then tracking inputs and outputs of energy, mass, metals, etc. provides the most meaningful way to explain and interpret the outcomes. Moreover, if the simulated population trends do not match up to reality (which we fully expect), flux tracking provides us with a more rigorous physical basis for adjusting the subgrid prescription. We will, for instance, be able to relate the energy and entropy injection from feedback *directly* to the propagation of metals and its impact on the metal census. This is more physical than comparing an artificial “high feedback” and “low feedback” parameterizations to the data. This is only one example of the improvements to physical interpretation that come from flux tracking, which make it so enabling of the “cosmological domain” that we aim for in this program.

5. Galaxy scaling relations and the evolving baryon census

One of the most important roles of theory is to provide physical insights into observed properties. Some of the most important observations of galaxies take the form of “scaling relations” that describe the interrelationships between galaxy mass, star formation rate, metallicity, size, and central black hole size. The surprising degree of clean behavior in these relations over 4 or more orders of magnitude in galaxy mass is interpreted as a deep regularity in the processes that form individual galaxies (e.g., Voit et al. 2015, 2017). Thus any theoretical effort to understand these underlying physical causes must eventually be able to produce populations of galaxies spanning the same range of properties as the observations. FOGGIE is already deriving important physical insights from its high-resolution approach to galaxy gas flows, but we will not really have compelling tests of this new approach until we can compare its results to the most powerfully diagnostic galaxy scaling relations. This consideration is a prime motivation for our plan to leap the gap between “zooms” and “cosmological domains” (Figure 1).

Our first goal will be to expand FOGGIE to a full cosmological domain so that population-wide comparisons are possible. To date, there exist no published galaxy scaling relations measured from ENZO “refine everywhere” simulations, with few AMR codes exploring the $z < 6$ regime of galaxy evolution for large cosmological volumes (though see, e.g., Ocvirk et al. 2008). Knowing where ENZO-E falls will help place the higher resolution zooms more commonly produced by these codes in context. We will measure the evolution of the commonly analyzed galactic scaling relations, including the galaxy stellar mass function, the stellar mass–star formation rate relation, gas fractions, the mass–metallicity relations, and size-mass relations for the full volume in FOGGIE:R.

Of particular interest is the evolving galactic baryon census, which combines the galaxy stellar mass function, ISM gas fractions, and the CGM content (Figure 6). Because of substantial halo-to-halo scatter, a large sample of halos is needed to robustly measure this and to trace its evolution through time. Do more gas-rich galaxies also have higher CGM gas masses, or are they gas rich because the CGM is gas-deficient? While existing simulations generally reproduce the observed stellar content of galaxies well (usually by construction) the way that they re-arrange the physical extent and thermal state of the CGM in order to do so differs dramatically from simulation to simulation. With our proposed simulations and the tool of flux tracking we will start to unravel the physical mechanisms by which galaxies process their gas in order to fill this parameter space. The baryon census is a fundamental observable that must be addressed by any simulation effort that aims to get at the deep physical processes of galaxy formation. The results in Figure 6 show that both SPH and moving-mesh codes have attacked this problem with mixed success. **Our proposed expansion of FOGGIE to FOGGIE:R in a full cosmological context is necessary to discover more spatially resolved and physically sophisticated treatments of the gas provide a solution to the unsolved problem of the baryon census.**

These measurements, both in general and for specific halos, will serve as benchmarks to compare against for our suite of subvolume exploratory simulations. Flux tracking will also enable these scaling relations to be directly comparable to analytic and semi-analytic models that make assumptions about how mass flow rates scale with galaxy or halo mass (e.g., Peebles & Shankar 2011; Shattow et al. 2015, Somerville & Davé 2015; Lu et al. 2015). This study will be led by the STScI postdoc, with some of the simulation analysis contributed by the MSU graduate student as part of their ramp-up to learning how to analyze ENZO-E simulations.

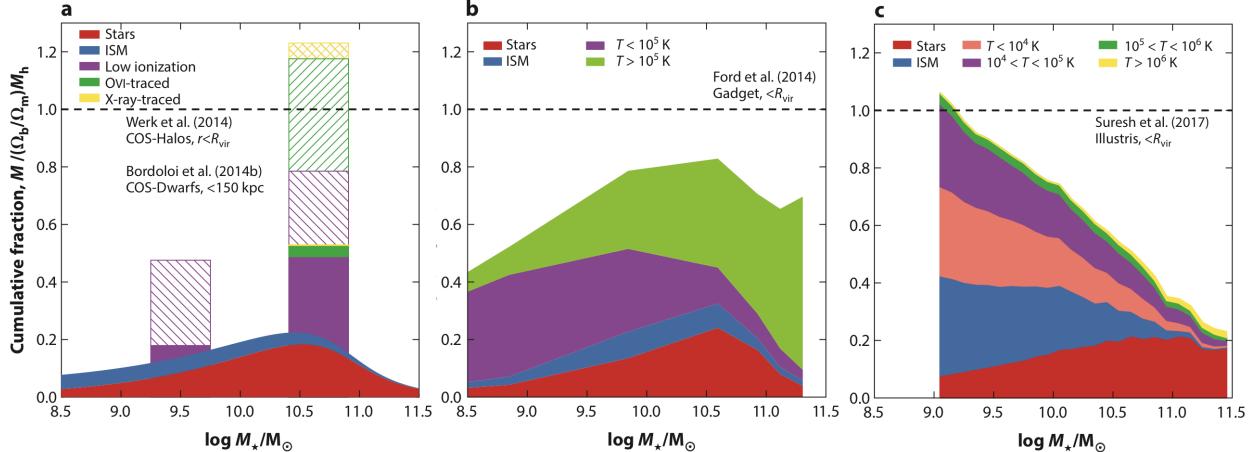


Figure 6. The baryon census in observations (a) and simulations (b; Gadget, and c; Illustris). While the simulations do a reasonable job at reproducing the stellar content of galaxies (by design), they disagree both with the observations and with one another with respect to the circumgalactic content. Figure adapted from Tumlinson, Peeples, & Werk (2017).

6. The evolving metal census and global circumgalactic statistics

While the evolving baryon census is sensitive to gas flows between the CGM and both the ISM and the IGM, the evolving metal census is an even more straightforward test of galaxy evolution models: as all metals are produced in stars and the deaths of stars, **the evolving metal census is more sensitive to flows from the ISM into the CGM (and back) and out to the IGM** (Figure 4). Moreover, galaxies' stellar metallicities are records of their history of gas phase metallicities, imprinting both their history of gas fractions and of metal loss via feedback (e.g., Peeples & Somerville 2013). Most of our observational tracers of the CGM itself is with metal lines, making the metallic content of the CGM easier to measure than the overall baryonic content (since HI is often saturated and thus metallicity corrections are difficult). Yet while most theoretical models and cosmological simulations do reasonably well at reproducing the observed *baryonic* content of galaxies, they are in broad disagreement when it comes to chemical evolution (Somerville & Davé 2015). Expanding FOGGIE into a cosmological volume with FOGGIE:R so that we can address the full metal census of galaxies is an important test of the feedback physics that distribute metals.

We expect two papers on the evolving metal census to be written in conjunction by the STScI group. The first will be an application of the flux tracking approach to understand the evolving metal census. The second will be an investigation of the circumgalactic ionic column density distribution functions (CDDFs) and how these absorbers relate to the underlying physical gas conditions. This is the sort of analysis that requires a full cosmological domain and will therefore help place the galaxy-centric census paper in a broader context.

6.1 Metals: Nature's tracer particles Our aim to understand the evolving metal census is threefold: (1) with the FOGGIE feedback prescriptions, how does the metal census plot evolve? (2) how and when do *individual* galaxies build up and redistribute their metals, i.e., what is the trajectory of individual galaxies in this space, and what clues do these trajectories give us to other processes of interest (mergers, AGN activity, environmental influence, and so on)? and (3) how does the observed (or inferred) metal census compare to the true metal census? Since the FOGGIE zooms concentrate on individual galaxies, we currently do not know how well FOGGIE's gas physics treatments will turn out on the mass-dependent metals census. Whether it succeeds or fails, we will want to know why, so we will use our flux tracking schemes to closely examine the dispersal of metals. Moreover, these tests and the

subsequent flux tracking interpretations (especially in the subvolume experiments) will help us choose which parameters to run the FOGGIE:ST simulation with—thereby hopefully improving FOGGIE’s modeling of the real universe.

6.2 The evolving circumgalactic distribution of metals As with the baryon census, one of our first tests will be to place FOGGIE:R in context will be measuring column density distribution functions for common ions (e.g., MgII). Observationally, dN/dz for strong MgII absorbers traces the cosmic star formation rate density (Matejek et al. 2013, Seyffert et al. 2013), while Ω_{CIV} increases steadily over cosmic time (Cooksey et al. 2013); this difference is often interpreted as MgII tracing recent outflows while CIV traces the overall enrichment of the universe. By “observing” the evolution of these two species (in addition to other low- and high-ions) both globally and within individual halos, we will better understand how these different species trace cosmic chemical evolution trends (Maiolino & Mannucci 2019).

A specific observational puzzle our simulations will uniquely address is that of the metallicity distribution of Lyman-limit systems (LLSs, i.e., gas with HI column densities of $>10^{16.2}\text{cm}^{-2}$; see, e.g., Lehner et al. 2019). LLS gas is generally found near galaxies, but galaxies “should” have polluted their near environs, making low-metallicity LLSs difficult to understand (Fumagalli et al. 2011). One solution is if pristine gas further from galaxies is able to, under the right circumstances, reach these relatively high densities. The low IGM resolution in current cosmological domain simulations, however, prevents this from ever happening. Likewise, another solution is for extremely low-metallicity gas to be able to reach the denser inner regions near galaxies, but at low-resolution, this gas will *always* be unphysically mixed and therefore polluted. With FOGGIE:R, we will statistically map the evolution of the metal content of the dense IGM and its relation to galaxies.

7. Angular momentum exchange and the evolution of galaxy morphologies

7.1 The observed kinematic and morphological evolution of galaxies At late cosmic times ($z < 1$, or the last 7 billion years), star-forming galaxies are typically thin, flat disks with high net angular momentum, while galaxies that have ceased forming stars are generally elliptical in shape with low net angular momentum. This clear dichotomy is but one example of how galaxy morphologies and kinematics relate to star formation rates, but the details of the why and how remain open questions.

Galaxies gain and lose angular momentum via exchange with their dark matter halos, the CGM, and mergers. Disks may form in part via gas accretion with high angular momentum, and preferentially low-angular momentum gas being lost via outflows (see Figure 4; Governato et al. 2010, Danovich et al. 2015). Observationally, there is some evidence for a connection between the orientation (and thus angular momentum) of galaxies and large-scale structure (Tempel et al. 2013ab); the wide-field surveys of the 2020s (such as *WFIRST*’s high-latitude survey) will place new constraints on how galaxies evolve in the cosmic web. *JWST* will unveil the morphologies, kinematics, and compositions of the gas and stars in galaxy populations in the early universe. *Euclid* and *WFIRST* will map distant galaxy morphologies across vast cosmic structures. These upcoming large-scale imaging and spectroscopic surveys will place new constraints on the alignment of galaxy structures with halos, filaments, and sheets over cosmic time. From a theoretical point of view, then, the kinematic evolution of galaxies must be approached holistically. We will adapt our flux tracking methods to account for the angular momentum exchange between stars, the ISM, the diffuse gas outside of galaxies, and dark matter.

7.2 Circumgalactic gas exchanges angular momentum with galaxies While the literature to date agrees that resolution is critically important to understanding the CGM itself, the impact of resolving the CGM on the galaxies themselves is not yet clear—the galaxies in these simulations change at about the same level found by changes caused by the butterfly effect (both in the FOGGIE zooms and, e.g., van de

Voort et al. 2019). On the other hand, there are *physical and numerical* reasons to expect the resolution of the low-density gas to effect how modeled galaxies evolve. For example, a simulation with increased spatial and mass resolution will also more finely sample the angular momentum distribution in the gas, and in the turbulent environment of the CGM this will more readily facilitate angular momentum exchange between fluid parcels, and thus the migration of low angular momentum gas onto the disk. Numerically, simulations with higher spatial resolution have lower effective viscosity, which substantially impacts the onset of turbulence and the transport of angular momentum between fluid elements. Taken together, **substantially increased CGM resolution has the potential to have a major impact on gas accretion onto and outflows out of the disk as well as its final distribution when it arrives there.**

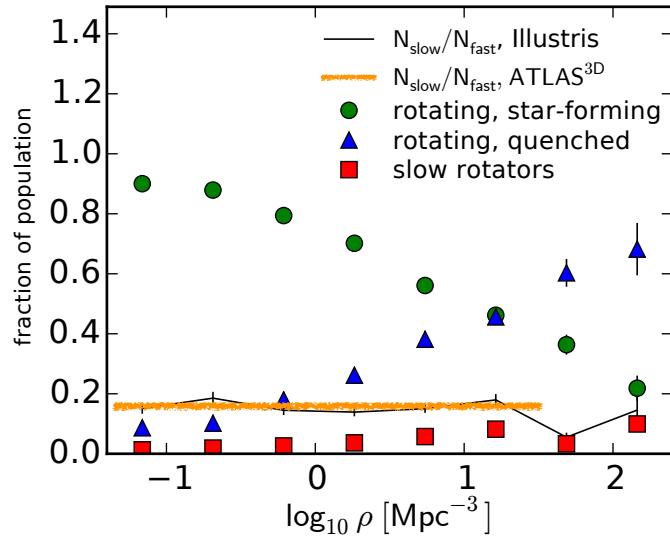


Figure 7: Environmental dependence of morphology and star formation in Illustris (Snyder et al. 2015), showing how cosmological assembly and angular momentum transfer leads to different galaxy morphologies in different environments. While such simulations broadly reproduce how galaxy properties depend on environment, they have not yet fully tested how galaxy morphologies and their alignment emerge from structure formation. With this program, we will probe how physics of the IGM and CGM affect the assembly of galaxies as a function of cosmic environment.

Previous generations of simulations have been in agreement that the angular momentum of circumgalactic gas depends on its temperature, with cold gas typically having a spin parameter $\sim 3\times$ that of the dark matter and the hot gas having a spin of only $\sim 2\times$ that of the dark matter (Stewart et al. 2017), but the simulations these results are based on are generally zooms, i.e., a relatively small number of halos. Moreover, the distributions of temperature, however, change when the resolution of the low-density gas is increased, in part because the gas can physically cool and in part because it is not forced to unnaturally mix. On larger scales, simulations suggest that galaxy structures' angular momentum should align themselves in specific ways with their large-scale structure (Welker et al. 2014; Dubois et al. 2014). Meanwhile, large-scale simulations have begun reproducing the observed trends of, e.g., the morphology-density relation, with feedback models tuned to reproduce the global star formation rate and halo occupation functions (Snyder et al. 2015; Figure 7).

7.3 Angular momentum tracking and observing morphological evolution We will therefore investigate how galaxy kinematics and halo spin parameters vary with respect to halo mass, star formation rate, redshift, and environment in the FOGGIE:R simulation. Taking it a step further, **we will use flux tracking to trace how both galaxies and the CGM gain and lose angular momentum as galaxy star formation histories evolve.** We will construct synthetic *JWST* and *WFIRST* data from which we will measure the same observable morphology metrics as in the real data, such as the disk size (Kravtsov 2013; Garrison-Kimmel et al. 2018) and H α rotation and velocity dispersion maps (Simons et al. 2019). We will use these synthetic data to calculate alignments between galaxy shapes and angular momenta with halos, filaments, and sheets. By doing so, we will determine the extent to which the physics of

the IGM and CGM affect galaxy morphologies and their relationship to cosmic structures. This work will be led by Co-I Snyder in conjunction with the flux tracking tools the postdoc will develop.

8. Concluding thoughts, team management, and proposed timeline

Large-scale cosmological simulations are now a mature approach to understanding the multifaceted physical effects that create galaxies. FOGGIE has demonstrated that high resolution in the gas flows is important to accurate recovery of the key observables. This effort began on isolated “zoom” galaxies to demonstrate feasibility of the calculations and significance of the results before expanding the approach to more typical “big box” simulations. We are now ready to take the first—and second—steps towards achieving this goal.

8.1 The FOGGIE collaboration The FOGGIE collaboration has been in place for three years; the Baltimore and MSU centers are in daily contact via Slack; we have weekly cross-institution group meetings and regular in-person collaboration meetings. PI Peebles manages the overall team, with Co-I O’Shea serving as the primary mentor and point of contact for students and postdocs at MSU. The STScI postdoc and MSU graduate student funded by this grant will have well-defined projects they can take ownership of in addition to being part of an established larger collaboration that includes observers, senior graduate students, and senior postdocs in addition to the Co-I’s here.

The STScI/JHU FOGGIE group leads the comparisons to and interpretations of real data, including generating and analyzing synthetic data in conjunction with the underlying physical properties in the simulations. The Baltimore group is responsible for the bulk of the development for running and analyzing our current suite of zoom simulations, and the STScI postdoc will be able to easily leverage these ongoing efforts for application to the cosmological domain simulations. Co-I O’Shea’s group at MSU is one of the core centers for ENZO-E development (from a large joint NSF CSSI grant), and is primarily responsible for implementing stellar and AGN formation and feedback algorithms in ENZO-E, as well as implementing new fluid and transport methods. The graduate student to be funded by this grant, Carlos Llorente, will have access to this expertise; he and Co-I O’Shea are well positioned to conduct the subvolume numerical experiments described in §2.3, interpret the results, and contribute to the design of the FOGGIE:ST calculation. As one of the ENZO-E core developers, Collaborator Smith will help with setting up the simulations, especially for the unusual numerical schemes we wish to explore in the subvolume experiments.

Finally, our group regularly mentors undergraduate students (via the MSU REU Co-I O’Shea is part of and the STScI SASP program the FOGGIE postdocs and the PI often mentor students through). These students will assist in testing code and making visualizations while being trained in numerical hydrodynamics, scientific writing, and giving science talks.

8.2 This grant’s timeline The relevant ENZO-E development will be completed before April 2020, when we expect our Pleiades allocation to start and for the PI to start running FOGGIE:R. Our anticipated timeline is:

Year 1: The STScI postdoc will write the first scaling relations paper, with contributions from MSU, and start developing the flux tracking analysis code. Co-I Snyder will start adapting our synthetic galaxy data codes to work for the new outputs. MSU will start running the subvolume suite of physics and numerics parameter space explorations.

Year 2: The STScI postdoc will apply the flux tracking method to understanding the evolution of the baryon and metal census. Co-I Snyder will adapt the flux tracking codes to also track angular momentum exchange. Llorente will write a paper on the results from the subvolume simulation experiments, with contributions from Baltimore.

Year 3: The PI will start running the FOGGIE:ST simulation. The STScI postdoc will finish the paper on the baryon and metal censuses, with contributions from MSU. Co-I Snyder will finish the paper on galaxy morphologies, kinematics, and angular momentum exchange with the CGM. The PI, Co-I Tumlinson, and the STScI postdoc will write a paper on the evolution of ionic CDDFs and how they relate back to the underlying changing physical conditions. Llorente will write a paper on the application of flux tracking to how AGN affect the CGM.

9. You might be wondering...

The CGM will still be more coarsely resolved than is shown to be important in the FOGGIE I & II papers. Isn't this a step back? No. It's a step towards the same goal but from a different direction.

Why not instead implement a “sub grid” model for the CGM at coarse resolution informed by higher-resolution simulations? The creation of sub-grid models are appropriate either when the physics or its phenomenology are reasonably well-understood (e.g., sub-grid models for turbulent energy dissipation and momentum diffusion), when there is a large separation between the spatial and temporal scales resolved in the simulation and the sub-grid process, and thus a coarse-grained or statistical approximation is appropriate (e.g., star formation and stellar feedback, AGN fueling and feedback), or when the physics of the sub-grid phenomenon is much more complex than can be practically modeled in the simulation and thus needs to be approximated (e.g., the plasma physics of stellar and AGN feedback). None of these criteria are relevant in our case, because the properties of the multiple phases of the CGM (e.g., ion structure) are closely tied to each other and their broader environment in ways that are not yet theoretically well-understood. Given that the observational phenomena that we wish to compare to will be *emergent* phenomena of all of these physical processes, using a sub-grid model would, effectively, be “garbage in, garbage out.”

Why a postdoc at STScI instead of a graduate student? The overall scope of science we want to do with these simulations right off the bat is too broad for a graduate student to pick up quickly while simultaneously learning how to set up, run, and analyze these large simulations. In particular, while we have flux tracking tools set up for analyzing our zoom simulations, the scale of these cosmological domain simulations will require massively parallel analysis tools to generate halo catalogs, merger trees, and other resulting data products. Perhaps most importantly, however, it will require substantial ability to plan data analyses and manage the deluge of data resulting from the analysis tasks. Thus, while the MSU grad student may learn this via the larger collaboration their work will be largely self-contained; the STScI postdoc will be more actively involved (and presumably leading) many aspects of the program.

Won't you need a lot of computing time to run these simulations? Yes, and we have requested the amount of time on Pleiades we will need to achieve our goals. Nonetheless, if need be, we will supplement it with computing time via NSF's XSEDE and PRAC programs, with the latter being the allocation method for Frontera (and the soon-to-be-decommissioned Blue Waters). PI O’Shea has led three successful PRAC programs, totaling more than 300 million core-hours on Blue Waters, and plans to submit a PRAC proposal supporting this project for Frontera. On the other hand, since ENZO-E is much less memory-intensive and scales more efficiently than ENZO, it will be able to use the available computational resources significantly more efficiently than current-generation cosmological codes. Our requested Pleiades allocation takes this into account and should suffice to support our science objectives.

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