Neutral Hydrogen in and around Galaxies in the SKA Era
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Looking to the future of simulations of H I

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Abstract. Atomic hydrogen (HI) gas is a key fuel reservoir for star formation in galaxies and provides an excellent tracer of their dynamical masses. The Square Kilometre Array (SKA) precursor observatories are already hinting at the incredible HI observations that we can expect from the SKA. We are also undergoing a quieter but equally exciting revolution in simulations of HI in galaxies. Up to now, we have had to resort to labelling HI in cosmological galaxy formation simulations in post-processing, subject to uncertain calibration and assumptions. New simulations are implementing cooling to 10 K and non-equilibrium ionization and chemistry, enabling on-the-fly calculation of HI fractions. We will soon have for the first time fully self-consistent, spatially-resolved predictions for the atomic hydrogen content, structure and kinematics of galaxies across cosmic history. I give an overview of the state of the art in simulation-based predictions for HI including recent breakthroughs and current challenges.

Keywords. simulations, atomic hydrogen, radio astronomy

These proceedings are closely based on a transcript of the conference presentation.

1. Introduction

The symposium organisers asked me to talk about simulations of H I, and in particular the future. Until I started writing my talk I didn't appreciate quite how difficult this was. I started thinking about when the first time that I heard about the SKA† was – that about 2009 I think, 15 years ago. People were already excited – it was going to be an amazing telescope. Then I tried to remember what simulations I was thinking about at that time. There was an exciting new project called GIMIC‡ (Crain et al. 2009). Readers with a long memory might remember that project, but it's no longer considered very relevant. This is all to say that the horizon for what's coming in the future of simulations is short – a couple of years, perhaps. I'll begin with giving my thoughts on why we make simulations, and then discuss some recent developments and things that I'm excited about coming from future simulations of H I.

Often you'll hear that "this simulation reproduces this or that scaling relation". It's useful to have a model that produces output that is reasonably realistic, but that's not the point of a simulation. In my opinion a simulation is for using to understand astrophysics and be able to pick apart a system in great detail. It's also useful as a tool to interpret what we see observationally. I say this to highlight that a lot of this talk is about the approximations that we use to work with H I in simulations. I've had many conversations over the years that begin: "the gas in these simulations isn't realistic enough". In a way that's right, it's not realistic: we're not simulating individual atoms, and that's never

† Square Kilometre Array
‡ Galaxies Intergalactic Medium Interaction Calculation

going to happen. The goal is to do the best that we can with the tools available to create something that we can study astrophysics with.

1.1. *Types of simulations*

As a (non-comprehensive) recap of the types of simulations that are available:

(1) Cosmological hydrodynamical simulations begin from initial conditions describing a periodic box filled with an almost uniform haze of dark matter and gas, with small fluctuations consistent with what we measure in the cosmic microwave background. This is evolved forward in time with gravity and hydrodynamics to produce an ab-initio galaxy formation simulation. An advantage of this approach is that lots of detailed physics can be included, while a disadvantage is that the calculations are very expensive and preclude the largest volumes and/or highest resolutions. Some examples include Remus et al. (2015); Schaye et al. (2015); Pillepich et al. (2018); Dubois et al. (2021); Hopkins et al. (2023).

(2) A computationally much cheaper calculation is a semi-analytic galaxy formation model. Here a galaxy is reduced to a system of differential equations representing the different gas reservoirs and stars, and the mass exchanges between them. More intricate variants might break a galaxy down into radial rings. At the cost of spatially resolving all of the detailed gas physics in the galaxies, many more of them can be simulated. It's possible to simulatie huge volumes encompassing statistical samples of galaxies, and to quickly explore a parameter space by running many model variations. Some examples include Somerville et al. (2008); Lacey et al. (2016); Lagos et al. (2018); Ayromlou et al. (2021).

(3) The last category that I'll mention are isolated hydrodynamical simulations. These don't start from a homogeneous box of gas modeling a representative piece of the Universe, but are instead set up 'by hand'. Gas (and potentially star) particles are placed in a disc within a halo of dark matter particles and the integration is started. Because they focus on a much smaller volume than a cosmological simulation much higher resolutions can be afforded. This approach also offers more control over the initial conditions. A disadvantage is that the initial conditions are set "by hand", in contrast with the ab-initio approach of cosmological simulations (of course this can instead be advantageous for some studies). Some examples include Marinacci et al. (2019); Lahén et al. (2020); Bieri et al. (2023).

2. Motivation for hydrodynamical galaxy formation simulations of H I

My discussion in this talk is biased towards cosmological hydrodynamical simulations because these are the kind of simulations that I work with most closely. (And they offer some of the best visualisations!) Why do we make these kinds of simulations? I've chosen some pictures here to highlight why this approach is particularly powerful in some contexts.

The MHONGOOSE† (de Blok et al. 2024) observation of the NGC 1566 field in the Dorado group of galaxies (Maccagni et al. 2024) evokes obvious interactions between the member galaxies (see their fig. 1). There are tails of gas, and asymmetric features that are clearly caused by galaxies flying past each other. Semi-analytic models generally fail to capture these features, and while it's possible to try to set up an interacting system in an isolated hydrodynamical simulation, this approach makes it very hard to understand the cosmological origin and rate of occurrence of interacting systems. Cosmological initial conditions produce interacting systems "for free" because galaxies form hierarchically

† MeerKAT H I Observations of Nearby Galactic Objects – Observing Southern Emitters

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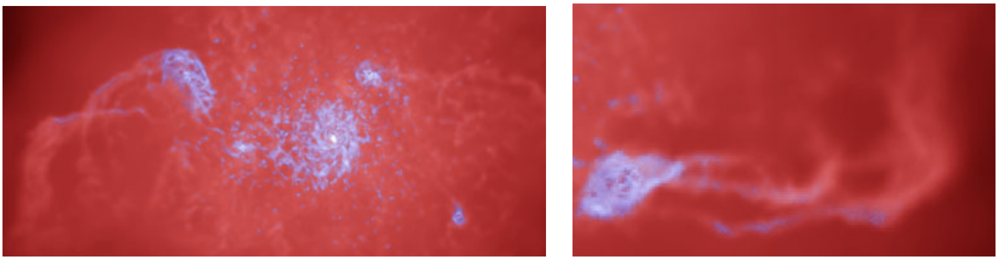

Figure 1. Two examples of galaxy interactions from the APOSTLE simulations. *Left:* An interacting group. The image shows gas density coloured by the density-weighted atomic hydrogen (H I) fraction such that ionized gas appears red and atomic gas blue. (There is a green channel for molecular gas but the contribution is too small to be visible.) *Right:* A satellite galaxy with a prominent H I ram pressure tail. Colouring as in left panel. Images created with PY-SPHVIEWER (Benitez-Llambay 2015).

and merge together. Fig. 1 (left panel) is an example from the APOSTLE† simulations (Sawala et al. 2016). This group of interacting galaxies has many of the same features seen in the MHONGOOSE observations. The image from the simulations pushes much further down in column density than what could be detected observationally. The faintest blue features are too diffuse to be observed with current instruments.

Observations of galaxy JW100 (Deb et al. 2022) reveal a ram-pressure tail being pulled off of it as it ploughs through the circumgalactic medium of its larger host, visible in both molecular gas and atomic gas (see their fig. 7). Fig. 1 (right panel) is again a simulation from the APOSTLE suite exhibiting a similar process. Such features are only obtained in the full hydrodynamic approach (in contrast to semi-analytic models), and again having interacting systems of galaxies that naturally arise in cosmological simulations is has advantages.

3. The future of simulations of H I

I'm next going to discuss two new breakthroughs in methodology that I'm excited about and are coming in new projects. I'll then present a case study exploring some of what I think will be fruitful approaches in coming years with one illustrative example. Finally, I'll highlight some of the challenges facing us in this field.

3.1. *New development: self-consistent H I on the fly*

The first new development that I want to mention is motivated by figures like fig. 1 from Crain et al. (2017) – a plot of the distribution of gas particle temperatures and number densities in a typical cosmological simulation from the past decade. There is gas from very high temperatures (10^8 K) through a cooling sequence, and at the bottom right of the plot there is a sequence of gas with a positive slope at around 10 000 K. In this simulation this latter sequence is what we interpret as atomic and molecular gas. In the real Universe atomic and molecular gas is much colder than this. Given the numerical parameters of this simulation, if the gas is allowed cool more than this it begins to artificially fragment. It would then form very dense clumps of stars, those stars would explode as supernovae and start to feedback energy into the gas, resulting in a very nasty non-linear coupled mess of, essentially, numerical errors. The compromise that has been conventionally used for many years now is to impose a temperature floor (or more correctly, a pressure floor) for the gas. Keeping it artificially pressurized prevents this artificial fragmentation and subsequent undesirable effects. An unfortunate consequence was that we then had to use

† A Project Of Simulations of The Local Environment

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empirically and analytically motivated prescriptions (such as Blitz and Rosolowsky 2006; Rahmati et al. 2013) to label gas as H I or H_2. This resulted in reasonably realistic H I distributions, but was always felt a bit uncomfortable – it was something that we had to live with and work around.

There's been a recent breakthrough in this area. It turns out that this artificial fragmentation comes from an interaction between two resolution scales in the simulations. The gravitational softening scale defines a length below which the stregnth of gravity is turned down to prevent two-body scattering. The hydrodynamic smoothing scale smooths gas properties on a different length scale: loosely speaking, the properties at a point in space are defined as a weighted average of the properties of neighbouring particles within the smoothing scale. These two scales interact, particularly around the Jeans' scale. As a reminder, the Jeans' length is defined as the length where the sound crossing time is equal to the gravitational free-fall time. In other words, if a gas cloud wants to collapse under its own gravity the Jeans' scale is the scale where pressure has a chance to prevent collapse because a pressure wave can cross the cloud in less than the free-fall time. If the hydrodynamics are over-smoothed (by choosing a smoothing scale that's too large), the pressure for example is smoothed out such that eventually it fails to resist gravitational collapse, leading to runaway collapse. The softening and smoothing scales can be controlled independently, giving some freedom to search for optimal combinations. The left panels of the left group in fig. 10 in Ploeckinger et al. (2024) shows an example of a galaxy simulated with the two scales set to similar values as in the EAGLE† (Schaye et al. 2015) project. There are many artificial clumps forming because here the gas has been allowed to cool below the pressure floor alluded to above. The clumps of gas are visible in the phase plot towards the right of the axes, in the region tinted red which is where the gas is expected to form these artificial clumps. The clumps themselves are highlighted in the upper panel. If different softening and smoothing scales are chosen, that still give a perfectly acceptable galaxy formation simulation, the regime where this numerical effect operates can be manipulated to entirely prevent the formation of artificial clumps. I think that people have understood this heuristically for a while now, for example there are adaptive softening schemes that largely circumvent the issue, but it wasn't understood in detail until the recent work led by Sylvia Ploeckinger (Ploeckinger et al. 2024). This paper gives clear guidance on how to choose resolution scales to avoid this numerical effect. The end result is that it's now possible to allow gas cooling to about 10 K and access the atomic and molecular gas regime much more directly and without artificial fragmentation. This means that it's now much more straightforward to label where the atomic and molecular gas is in a simulation, without resorting to prescriptions such as those of Blitz and Rosolowsky (2006); Rahmati et al. (2013).

3.2. *New development: non-equilibrium chemistry*

The second new development that I want to highlight is recent work in non-equilibrium chemistry. The simplest approach to hydrogen (for instance) chemistry and ionization state in a simulation is to assume that any given element of gas in ionization equilibrium. Given the local ionizing radiation field, gas temperature & density and so on at a location, the equilibrium ionization and molecule formation state of the gas can be computed. However, things are not always in equilibrium. The radiation field might suddenly ramp up and start to ionize the gas, for example, but it takes the gas time to react and re-equilibrate. Alex Richings in particular (Richings et al. 2022) has done a lot of work on non-equilibrium chemical networks. The CHIMES module (Richings et al. 2014a,b) follows 157 different molecules and ions, and a very large number of reactions. What

† Evolution and Assembly of GaLaxies and their Environments

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are the consequences for gas in galaxy simulations? Fig. 14 in Richings et al. (2022) illustrates this. This again shows the gas phase diagram – temperature versus density – but zoomed in on low temperatures and high densities (the atomic and molecular gas regime) relative to examples cited above. The upper panels show where H I and H_2 occur in this space: anywhere that's yellow in the top left has abundant H I, and the highest densities and lowest temperatures are in yellow in the right panel where H_2 forms. The lower panels compare the distribution of gas in this space in the equilibrium and non-equilibrium cases. In the lower-left panel for example the regions coloured red are those where there is more H I than would occur in the equilibrium case when non-equilirbium effects are accounted for, while blue shows a relative deficit. The same thing for H_2 is shown in the lower-right panel. For H_2 the differences are obviously large, but notice that the colour scale shows the logarithm of the ratio – up to a factor of 1000. H I looks at a glance like it has much smaller differences, but any region that's even slightly red or blue already represents a discrepancy of a factor of a few. I think that these differences becomes particularly important when seleting subsets of gas. A galactic fountain or an accretion flow, for example, probably occupies a particular region of the phase diagram, and it wouldn't be surprising to find that this is where non-equilibrium effects become very important. I think that there's a lot of work to be done to understand the consequences of chemical/ionization non-equilirbium effects for galaxies in simulations, but I also think that there's a lot of potential to learn some interesting new things.

3.3. *Case study: a hybrid hydrodynamical + semi-analytic approach*

I'd next like to present an illustrative case study highlighting the importance of doing hydrodynamic simulations and how some of their limitations can be mitigated with the help of semi-analytic models. First, a brief reminder of a quantity often encountered in H I astronomy: w_{50}, the full width at half-maximum of the H I line of a galaxy. The classical spectral shape, particularly for massive galaxies, is a two-peaked, "double-horn" profile. The two peaks come from the outer edges of the approaching and receding sides of an (inclined) disc. Since the rotation of the disc sets the width of the spectral line w_{50} is a good, although biased and limited, tracer of the dynamical mass of a galaxy.

We can count sources (galaxies) as a function of either their H I masses (upper left panel of Fig. 2) or their H I line width (upper right panel). This figure is made from an output of the GALFORM semi-analytic model (Lacey et al. 2016; Brooks et al. 2023): a simulation containing only dark matter has each halo populated with a simplified model of a galaxy. We assume that those galaxies have a line width determined by the mass profile of the galaxy and a constant-density disc model for the H I. Measurements from the ALFALFA† survey are plotted for comparison. The simulation is a poor match to the measurement, especially for the line width function. (The stregnth of this particular simulation – Sawala et al. 2022, – is that it reproduces the detailed large-scale structure in the nearby Universe, so we learned a lot about survey systematics from this project but had to work around this very poor match to the data.) The lower panels of Fig. 2 are similar to the upper panels, but for a hydrodynamical simulation, in this case the EAGLE model (Schaye et al. 2015). This reproduces the observed line width function much more closely. The reason for this is that reproducing the line width function requires accounting for the "messy" gas kinematics that arise in galaxies, such as in warped, disturbed/perturbed and interacting galaxies, as well as galaxies blended with their satellites. The match is not perfect, at the low-velocity or the low-mass end especially. This is mostly a consequence of the pressure floor alluded to above, so I expect this to improve in the near future.

† Arecibo Legacy Fast ALFA (Arecibo L-band Feed Array)

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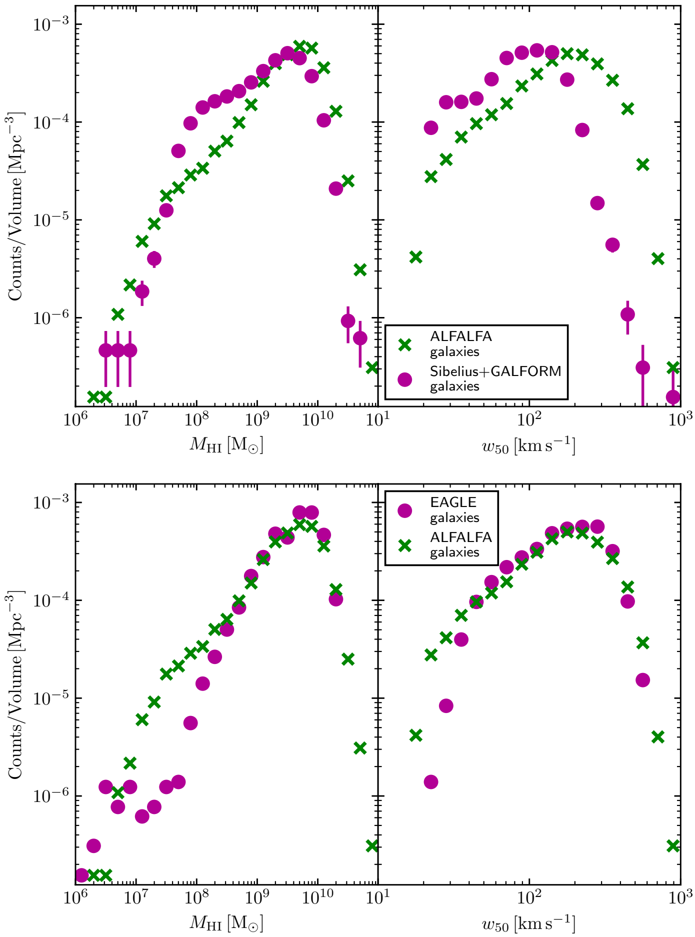

Figure 2. H I mass functions and width functions from observations and simulations. *Upper left:* Number density of detected sources as a function of H I mass M_{HI} in the ALFALFA survey (green crosses) and in an ALFALFA-like survey constructed from the SIBELIUS simulation and GALFORM semi-analytic galaxy formation model (purple points). *Upper right:* As upper left but showing the number density of detected sources as a function of H I line width, w_{50}. *Lower left:* as upper left, but comparing the ALFALFA survey (green crosses) and an ALFALFA-like survey constructed from the EAGLE hydrodynamical galaxy formation simulation (purple points). *Lower right:* as lower left but showing the number density of detected sources as a function of w_{50}. Refer to Brooks et al. (2023) and Oman et al. (2024) for further details of the calculations leading to the upper and lower panels, respectively.

There's also a sudden truncation at the high-mass or high-velocity end: because this is an expensive hydrodynamical simulation large volumes are prohibitively expensive, so the rarest high-mass sources don't occur in the relatively small volume simulated. There's an opportunity to blend these two approaches, semi-analytic and hydrodynamical, together. I could imagine taking the results of a hydrodynamical simulation to produce a library of spectra that is then used to statistically populate dark matter halos in a much larger volume, assisted by a galaxy catalogue from a semi-analytic model. This could be a practical way to realise simulations covering the very large volumes (relative to what's achievable with high-resolution hydrodynamical runs) needed to compare with the very large surveys coming soon or now underway (e.g. Braun et al. 2015; Koribalski et al. 2020), without sacrificing the detailed physics included in the small-volume hydrodynamical simulations.

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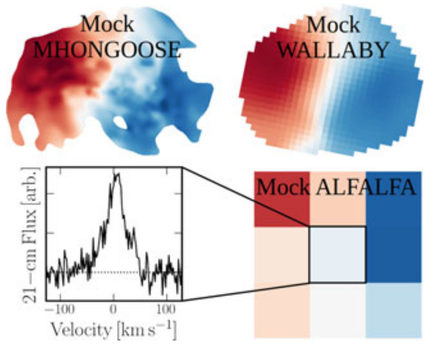

Figure 3. Simulated observations of H I velocity fields of a dwarf galaxy at a distance of 4 Mpc as seen by a telescope with a resolution similar to that used in the MHONGOOSE survey (upper left), the WALLABY survey (upper right) and the ALFALFA survey (lower right). In the latter case the galaxy is spatially unresolved, but is spectrally resolved (lower left). The velocity fields are truncated where the column density drop below about $1\,\mathrm{M_\odot\,pc^{-2}}$. Mock observations created with MARTINI (Oman 2019, 2024).

3.4. *A scientific challenge: putting simulations on even footing with observations*

It has become clear to me over time that making comparisons between simulations and observations in a fair way is very important. It's all too common to see years of work put into obtaining data, reducing them, analysing them, finally writing the manuscript, and then suddenly – it's time to compare with simulations, so some predictions are quickly extracted and added to a plot, a couple of paragraphs of interpretation are written, and little is learned. In practice I think that it's usually much more productive to make the exercise of comparing with simulations into "paper two" (or an integral part of the work from the beginning).

Casting theoretical predictions into the same "language" as observational data is a lot of work. I want to stress that it's probably best to have people involved coming from both sides – simulations and observations – to work through the effort of making mock data products from the simulations so that truly apples-to-apples comparisons can be made. Fig. 3 was made with my MARTINI† software package (Oman 2019, 2024). It highlights that comparisons to for, example, the MHONGOOSE survey (de Blok et al. 2024) versus the WALLABY‡ survey (Koribalski et al. 2020) versus a low-resolution survey like ALFALFA (Haynes et al. 2018) require qualitatively different data products to be produced from the "raw" simulation outputs. These are all observations of the same galaxy! Taking "the simulations" as making a single, monolithic prediction does not lead to fair, correct comparisons.

3.5. *A technical challenge: the rise of the GPU*

I'll briefly touch on a technical challenge that's on the horizon. Supercomputer systems have started to appear that have a large fraction of their computing power in graphics processing units (GPUs). Fig. 4 (based on `https://top500.org/statistics/overtime/`) shows the prevalence of top systems with more than 90% of their cores in the form of GPUs over time. I think that as a field we're not really prepared for this. There is some

† Mock Array Radio Telescope Interferometry of the Neutral ISM (InterStellar Medium)
‡ Widefield ASKAP (Australian Square Kilometre Array Pathfinder) L-band Legacy All-sky Blind surveY

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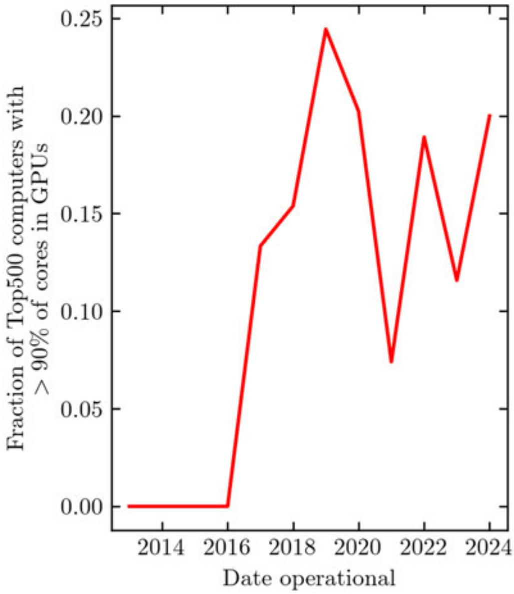

Figure 4. Fraction of high-performance computing (HPC) systems from the Top-500 (https://top500.org) list with 90% or more processing cores in the form of graphics processing units (GPUs) or tensor processing units (TPUs), as opposed to central processing units (CPUs), as a function of time. Systems with large fractions of GPUs/TPUs have begun to appear in the past decade.

discussion along the lines of "all of these GPUs are available, we should probably try to use them", but it feels to me like this is not because GPUs are ideally suited to the calculations that we want to do. Instead there's a sense of possible panic because of the risk that GPUs replace CPUs in supercomputers, making it necessary to use them whether they are suited to the calculations or not. It's worth highlighting that GPUs can be very energy efficient relative to CPUs, providing another interesting dimension to explore in this area.

4. Conclusion

It's important to remember that we're in the transition from the first into the second generation of hydrodynamical simulations that broadly reproduce observed populations of galaxies. I think that there is still a lot to come from this field. The ceiling is very high, which is exciting. I'm also personally very excited to start working with simulations of size and resolution to be a good match to the surveys that the SKA in particular is going to produce. As a final thought, I encourage theoreticians to work closely with their observer colleagues, and observers to work closely with their theoretician colleagues – this is the way that we can make the most of simulations of H I.

5. Transcript of discussion

A. Ponomareva: Thank you very much it was a fantastic talk it was amazing to see. I wanted to touch on your last take-away point and also connect the two talks that we've just heard. What, as a simulator, are you most excited about from the new surveys that are coming? Are there any particular theories that you want to test? Do you want higher redshift, or smaller galaxies? What's most exciting from the new H I observations that are coming up?

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K. Oman: I'll give it my own bias. I'm most excited about pushing down in column density and in mass. Kristine [Spekkens] was talking about the very faint circumgalactic gas. I think that's very exciting and MHONGOOSE is already giving some interesting hints that simulations might not look so much like what we're observing. Also those very low-mass galaxies. Finding an H I cloud without stars in it, that would be very interesting indeed. There have been some claims, I think a bit optimistic, for detections of those kinds of objects. If we look deep enough we still always tend to find stars, but hopefully in the next 10 years or so we can start to find some of those objects.

N. Katz: Thanks for a really interesting talk. But I think that we as theorists, especially in these audiences that are so observationally dominated, are a little over-optimistic and dishonest in how good our simulations actually are. For example, you showed adding this physics of the chemistry networks. That sounds great in principle but we're really orders of magnitude away from resolving the scales that we know those processes really take part in. And one thing that you skipped over, for example, is AGN and supernova feedback. Those dominate all of these simulations. But again we're orders and orders of magnitude away from really resolving these proceeses. We show plots of how we match all of these observations, either how these galaxies look or the number counts that you showed. But the different simulations are matching these things, yet the physics that's going on inside these simulations and how they include some of these subgrid physics is completely different across these simulations. So I think that the observers should realize that we're really not that able to make concrete predictions of these different processes. I think we're hyping up a little bit how well we can actually do. Personally, I think that the only way forward is to put in subgrid models since I don't think any time in the near future we'll have the resolution to resolve any of these processes. I'd like to ask what your opinion is on that.

K. Oman: I tried to air a bit of the dirty laundry in the talk and mention some of the things we've been struggling with, while keep it optimistic by showing some of the recent advances. But, everything that we do is formally unresolved. All of these processes – supernova feedback, AGN feedback, star formation even – different simulations use different approaches, and they make complementary predictions. In the first slide of the talk I said that "The point is not to reproduce reality, the point is to understand something about astrophysics." Hopefully most of us in the theory community understand the limits of our models and also how to productively get things out of them – otherwise we wouldn't make the simulations in the first place. I tried to close on the idea that we don't want to take the predictions of the simulations blindly and compare them naively. It's about having a productive conversation between the people who really understand the measurements coming out of the telescopes and the people who really understand the predictions coming out of the simulations, and putting that together to try to learn something.

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