

Title: Modeling high redshift structure formation and reionization

Speakers: Rahul Kannan

Series: Cosmology & Gravitation

Date: February 21, 2023 - 11:00 AM

URL: <https://pirsa.org/23020019>

Abstract: One of the exciting new frontiers in cosmology and structure formation is the Epoch of Reionization (EoR), a period when the radiation from the early stars and galaxies ionized almost all gas in the Universe. This epoch forms an important evolutionary link between the smooth matter distribution at early times and the highly complex structures seen today. Fortunately, a whole slew of instruments that have been specifically designed to study the high-redshift Universe (JWST, ALMA, Roman Space Telescope, HERA, SKA, CCAT-p, SPHEREx), have started providing valuable insights, which will usher the study of EoR into a new, high-precision era. It is, therefore, imperative that theoretical/numerical models achieve sufficient accuracy and physical fidelity to meaningfully interpret this new data. In this talk, I will introduce the THESAN simulation framework that is designed to efficiently leverage current and upcoming high redshift observations to constrain the physics of reionization. The multi-scale nature of the process is tackled by coupling large volume ( $\sim 100$ s Mpc) simulations designed to study the large-scale statistical properties of the intergalactic medium (IGM) that is undergoing reionization, with high-resolution ( $\sim 10$  pc) simulations that zoom-in on single galaxies which are ideal for predicting the resolved properties of the sources responsible for it. I will discuss applications from the first set of papers, including predictions for high redshift galaxy properties, the galaxy-IGM connection,  $\text{Ly-}\alpha$  transmission and back reaction of reionization on galaxy formation. I will finish by highlighting recent improvements to the model and proposed future work.

Zoom link: <https://pitp.zoom.us/j/94595023029?pwd=b0c0MVZHZ01rQnprS1ZCSzVIZktqUT09>

THESAN

# Modeling high redshift structure formation and reionization

**Rahul Kannan**  
York University

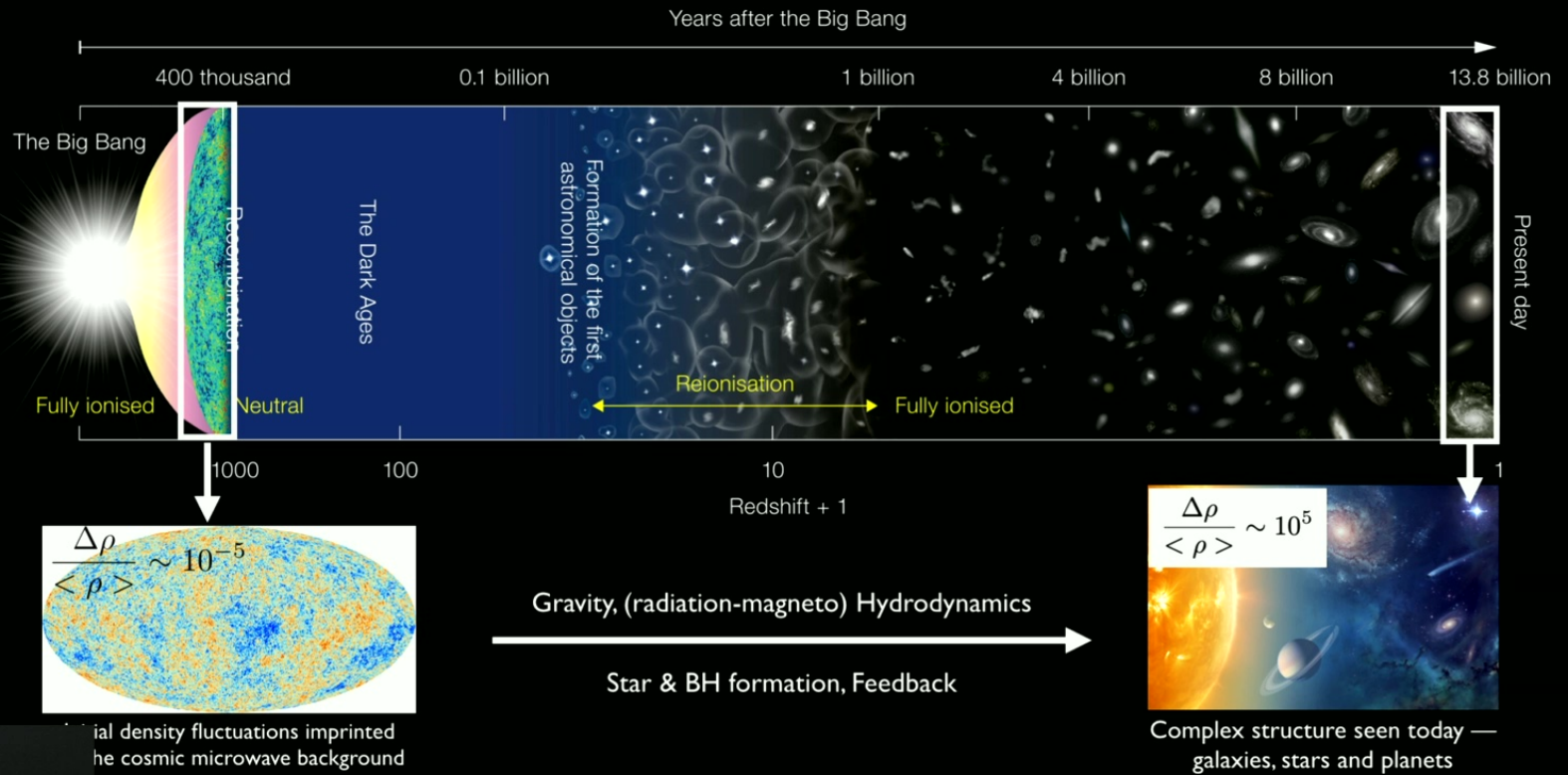
Cosmology Seminar  
Perimeter Institute for Theoretical Physics  
February 21, 2023



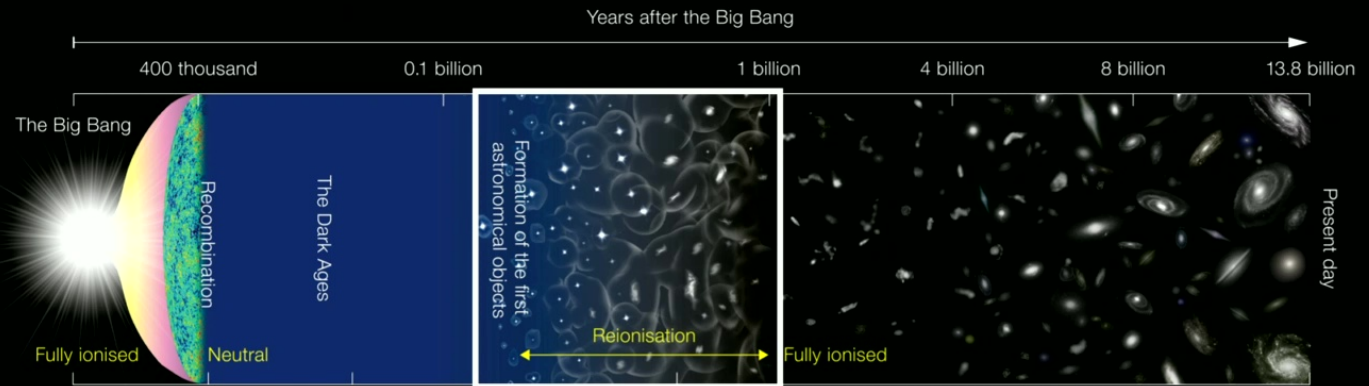
**$z = 7.00$**   
Cosmological Redshift

**765 Myr**  
Time Since Big Bang

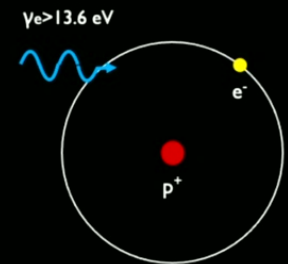
# Cosmological structure formation



# Epoch of Reionization (EoR)



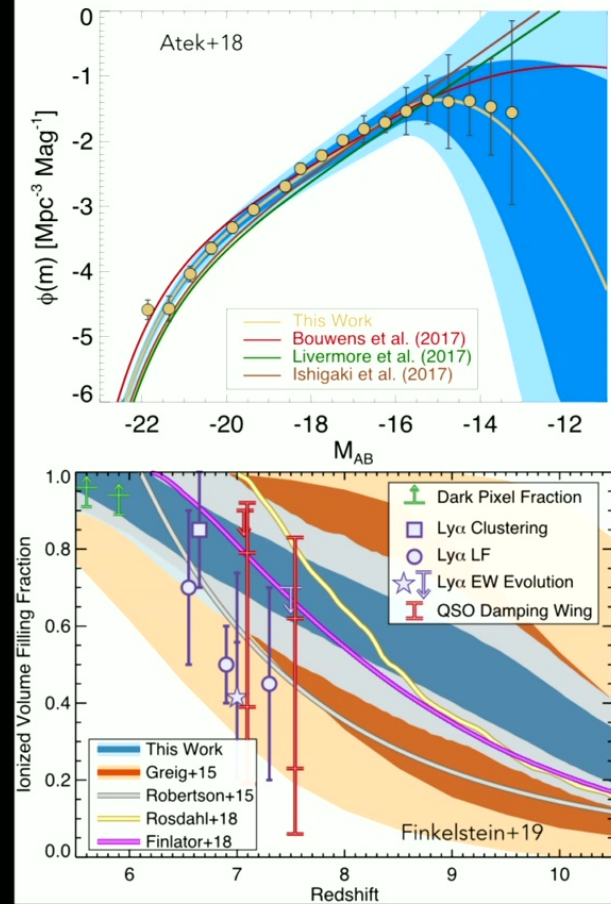
- Epoch of Reionization  $z=15-5$  - Universe undergoes a phase transition
- All photons with energy  $> 13.6$  eV have the ability to ionize hydrogen
- Radiation from first stars and galaxies ionizes the neutral Hydrogen in the universe and heats up the gas to  $\sim 10,000$  K





# Epoch of Reionization

- What are the sources responsible for Reionization?
- When did Reionization happen?
- What is the duration of this process?
- Can we constrain cosmology and understand the physics of structure formation using Reionization?



# Simple model for reionization

Assume every neutral Hydrogen atom requires one ionizing photon ( $>13.6$  eV)

$$N_{\gamma} = N_{HI}$$

We also need to account for recombinations, i.e., high density hydrogen atoms recombine and therefore need more than one photon to fully ionize it

$$N_{\gamma} = N_{HI} \left( 1 + \int_0^t \frac{dt}{t_{rec}} \right)$$

# (Not so) Simple model for reionization

(accounting for time and spatial variation in the reionization process)

Depends on the source distribution  $f(x,t)$   
Mainly stars and AGN

$$N_{\gamma}(x, t) = N_{HI}(x, t) \left( 1 + \int_0^t \frac{dt}{t_{rec}} \right)$$

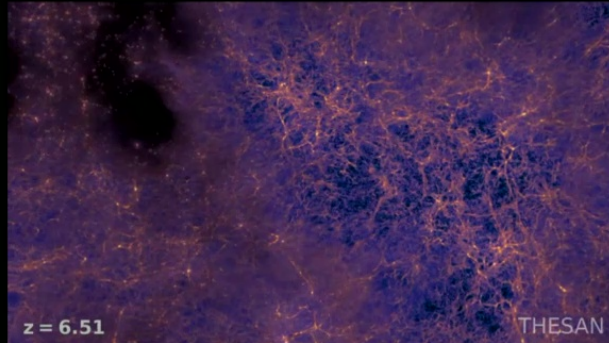
Depends on cosmology and the  
Reionization process itself

Depends on the matter distribution in  
the Universe and the physics of  
cosmological structure formation

Each of these simple terms is a complicated function of the underlying cosmology and the astrophysical processes affecting structure formation

# Reionization is a complex multi-scale problem

Stars (GMCs) and BH generate photons ( $\sim \text{pc}$ )



Transmission through ISM ( $\sim \text{kpc}$ )



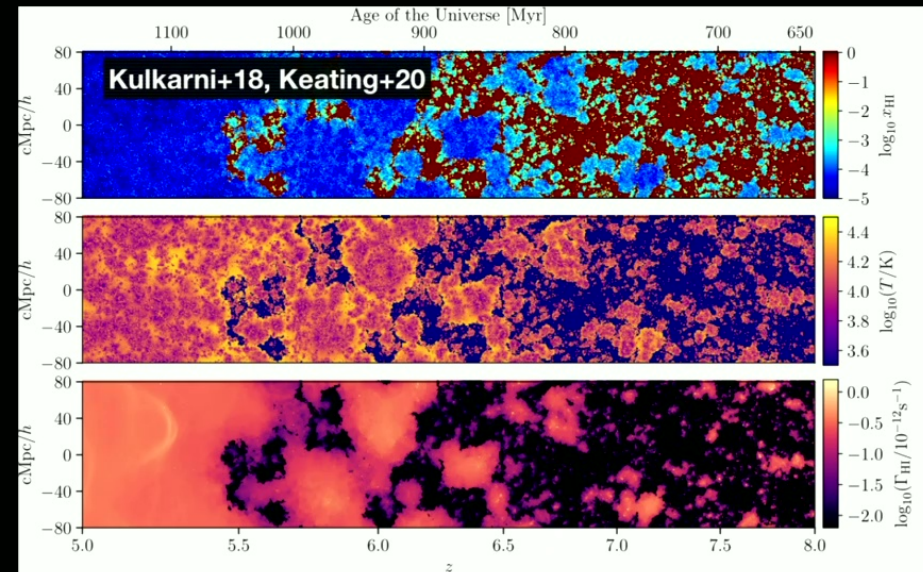
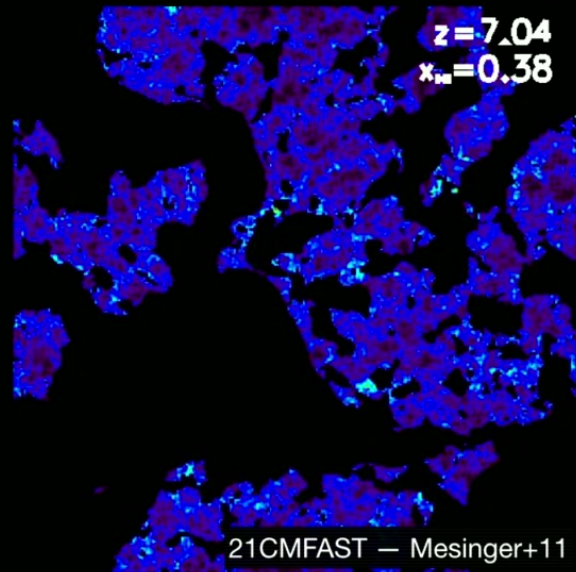
Transmission through CGM ( $\sim 100\text{s kpc}$ )



Affect on IGM ( $\sim 100\text{s Mpc}$ )



# Widely used EoR models



- Semi-numerical / post process RT
- efficient parameter exploration
- approximate source functions, escape fractions, clumping factors, etc.
- Imprecise radiation-gas coupling - inability to model self-shielded systems which bias 21cm (Cain+16, Georgiev+21) and mean free path estimates (Cain+21, Davies+21)

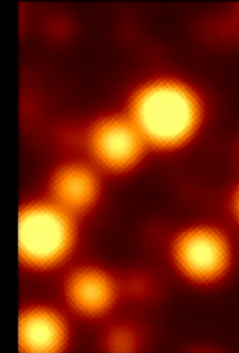


# High-z observations - new high precision era

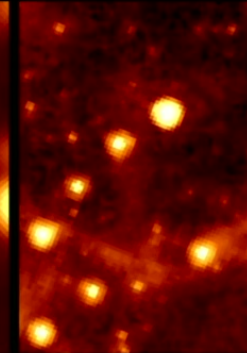


JWST

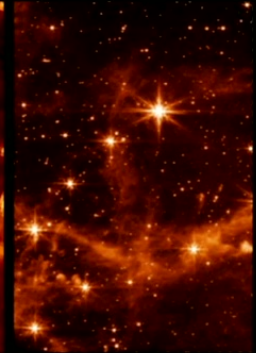
ALMA



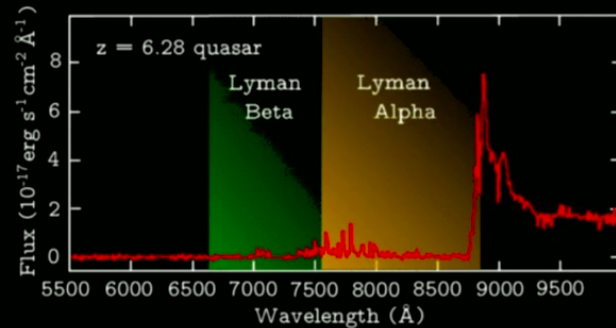
WISE W2 4.6  $\mu\text{m}$



Spitzer/IRAC 8.6  $\mu\text{m}$



JWST/MIRI 7.7  $\mu\text{m}$

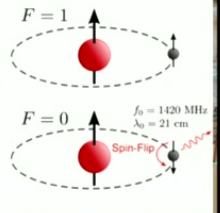


Intensity  
mapping

21cm &  
Nebular  
lines



HERA/SKA/LOFAR

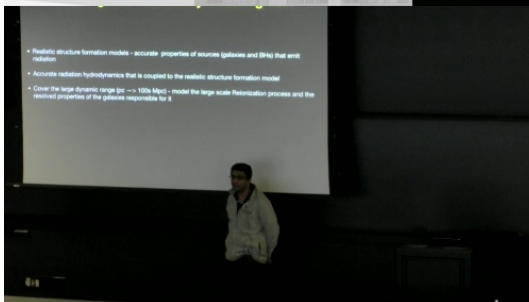


There is therefore the need for high fidelity theoretical models to accurately interpret these observations and make accurate predictions



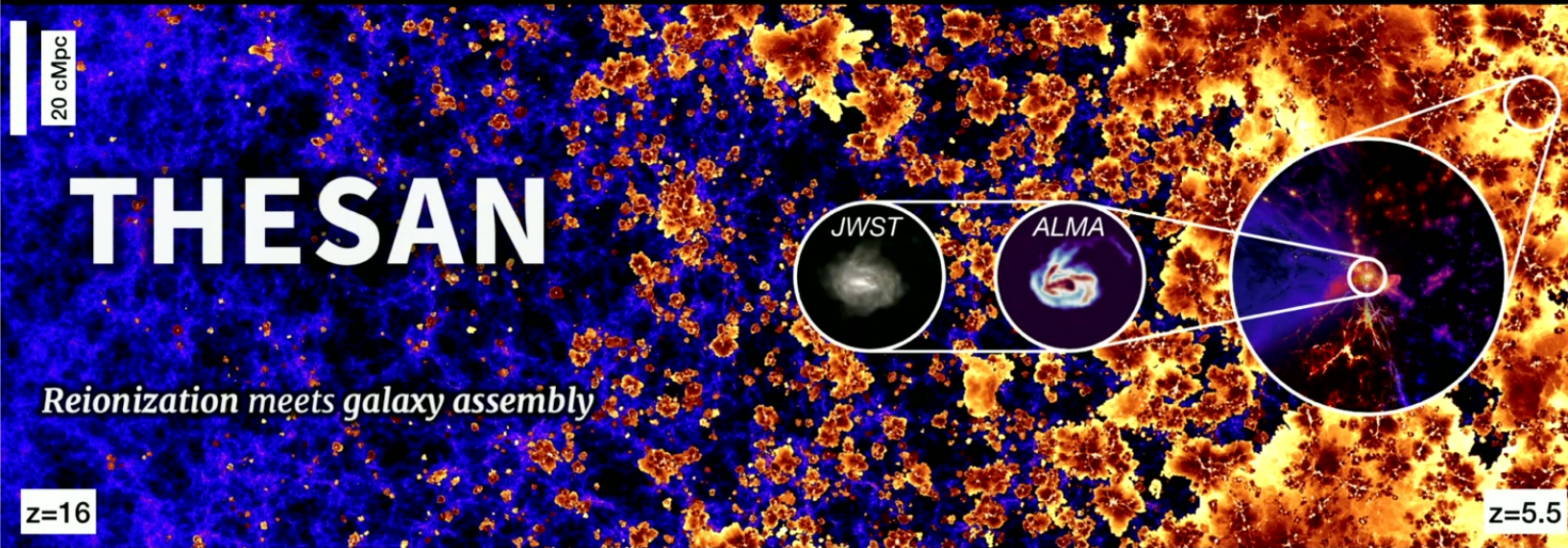
# Challenges for accurately modeling EoR

- Realistic structure formation models - accurate properties of sources (galaxies and BHs) that emit radiation
- Accurate radiation hydrodynamics that is coupled to the realistic structure formation model
- Cover the large dynamic range (pc  $\rightarrow$  100s Mpc) - model the large scale Reionization process and the resolved properties of the galaxies responsible for it





# The THESAN Project



*Reionization meets galaxy assembly*

Large volume — high resolution — coupled reionization and galaxy formation simulations

Team Lead: **Rahul Kannan**

Enrico Garaldi, Aaron Smith, Rüdiger Pakmor, Volker Springel, Mark Vogelsberger & Lars Hernquist

**Kannan+22a,b; Garaldi,Kannan+22; Smith,Kannan+22**





# The THESAN Project

Subscribe

Latest Issues

SCIENTIFIC  
AMERICAN®

Cart 0 Sign In

**COVID** Health Mind & Brain Environment Technology Space & Physics Video Podcasts Opinion Store

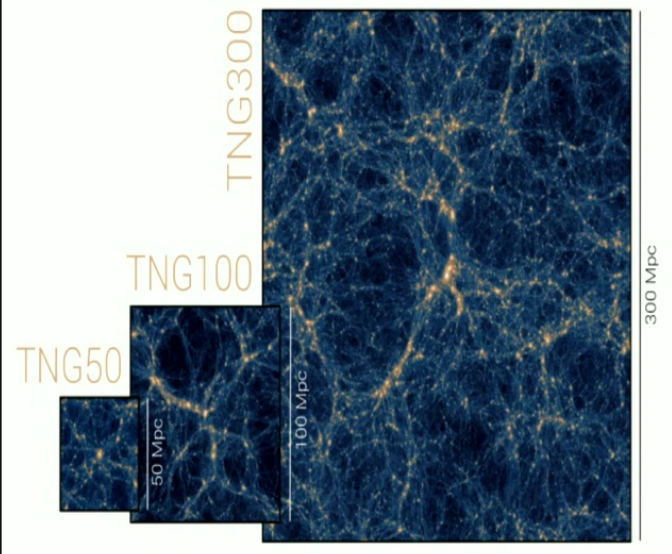
COSMOLOGY

## New Record-Breaking Simulation Sheds Light on ‘Cosmic Dawn’

THESAN—the largest, most detailed computer model of the universe’s first billion years yet made—is helping set expectations for observations from NASA’s James Webb Space Telescope



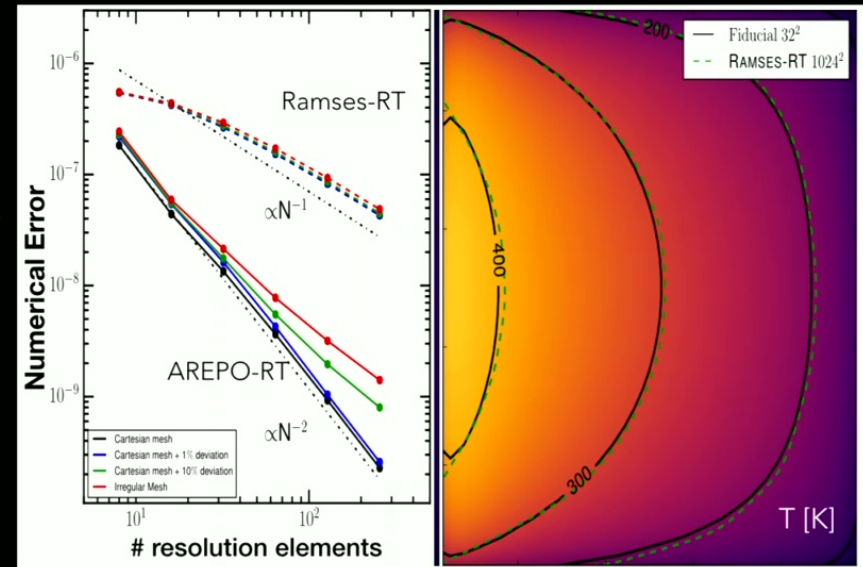
# Accurate galaxy formation model + RHD



IllustrisTNG  
(Springel+18)

- Well tested galaxy formation model, works extremely well down to  $z=0$

+



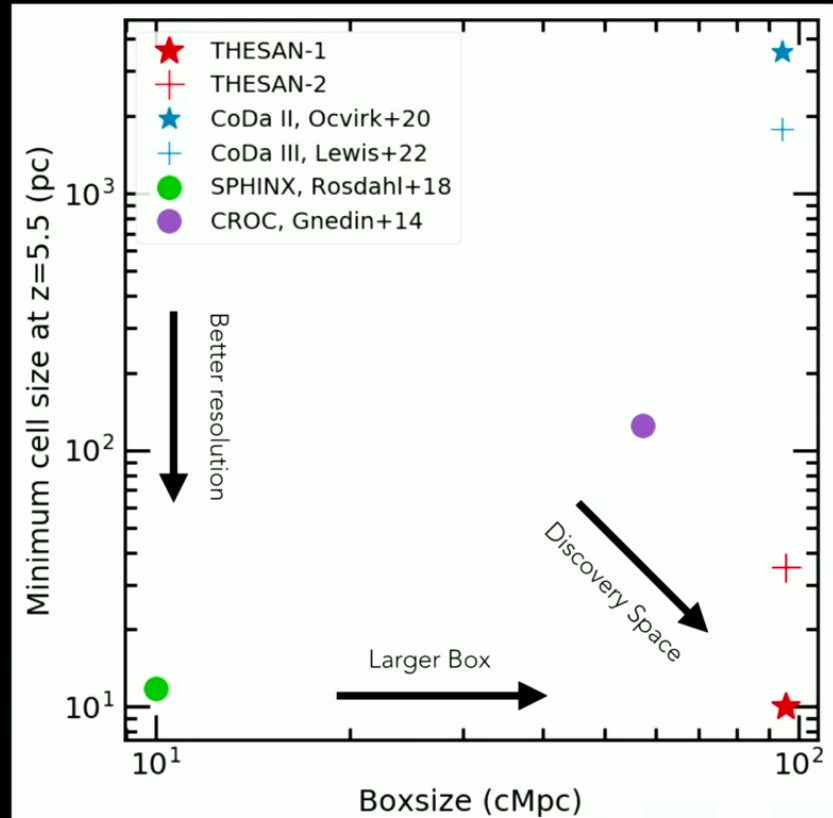
AREPO-RT  
(Kannan+19)

- Efficient and highly scalable radiation hydrodynamics module that solves the RT equations on the native Voronoi Mesh

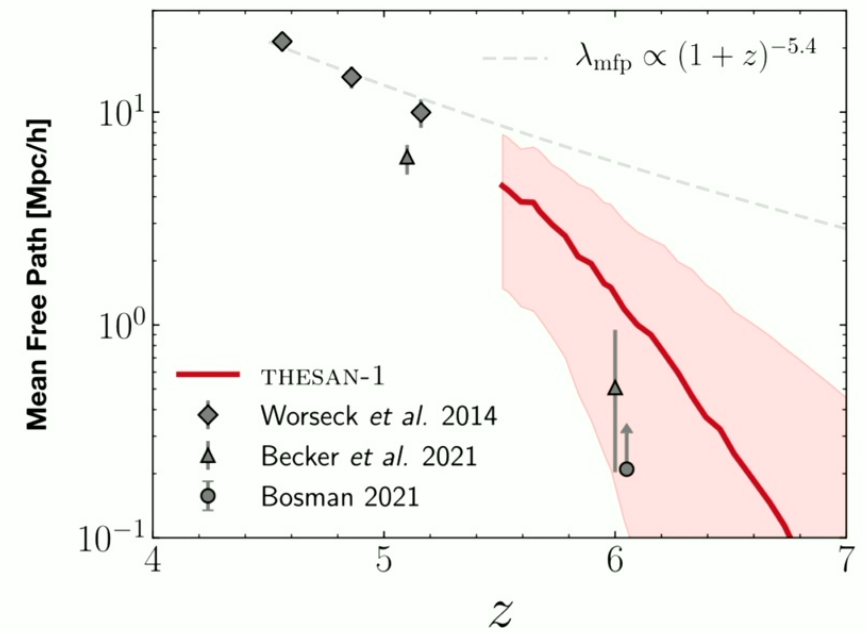
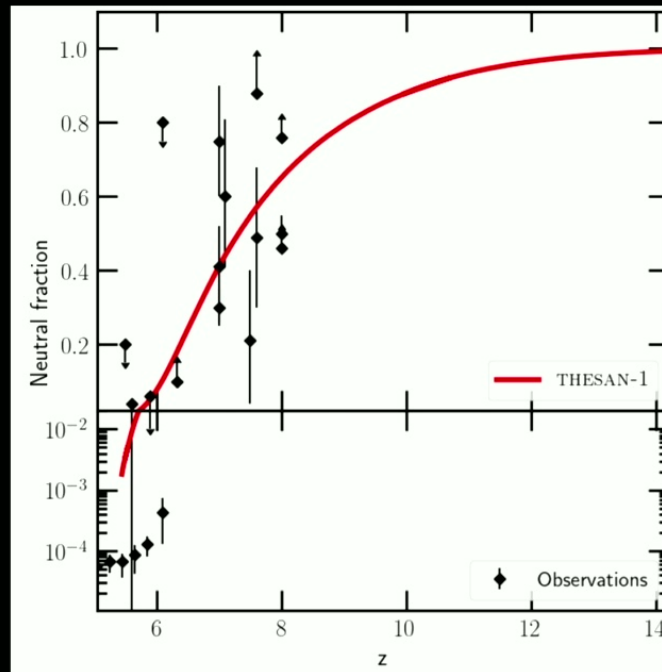


# The THESAN Project

- Large volume simulations (95.5 cMpc)<sup>3</sup>
- Resolves atomic cooling halos throughout the simulation volume
- Performed on 57,600 cores on SuperMUC-NG
- Significant step forward in modeling EoR



# Accurate Reionization History



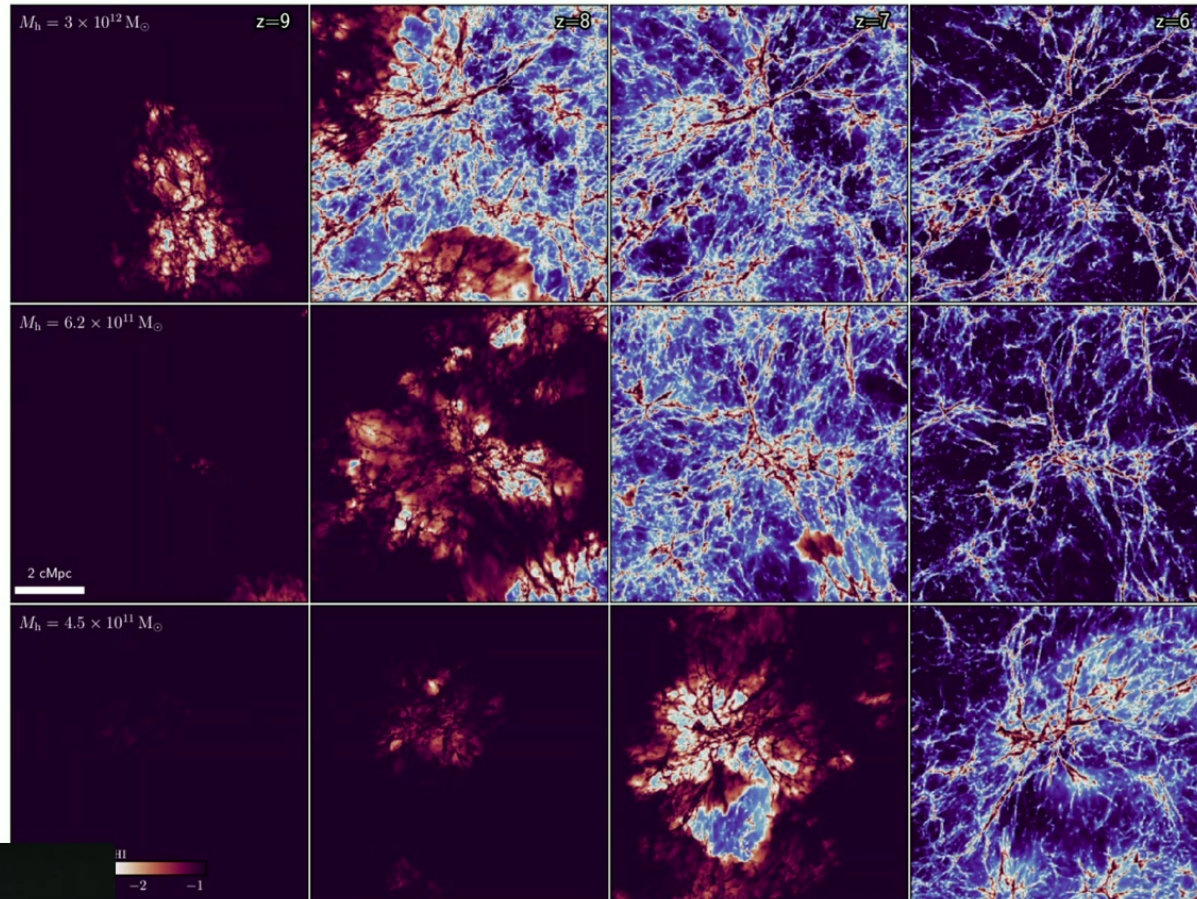
Kannan+22; Garaldi, Kannan+22

- Matches ionization history

model rapid mean free path evolution without resorting to sub-grid sink models (Cain+21, Davies+21)







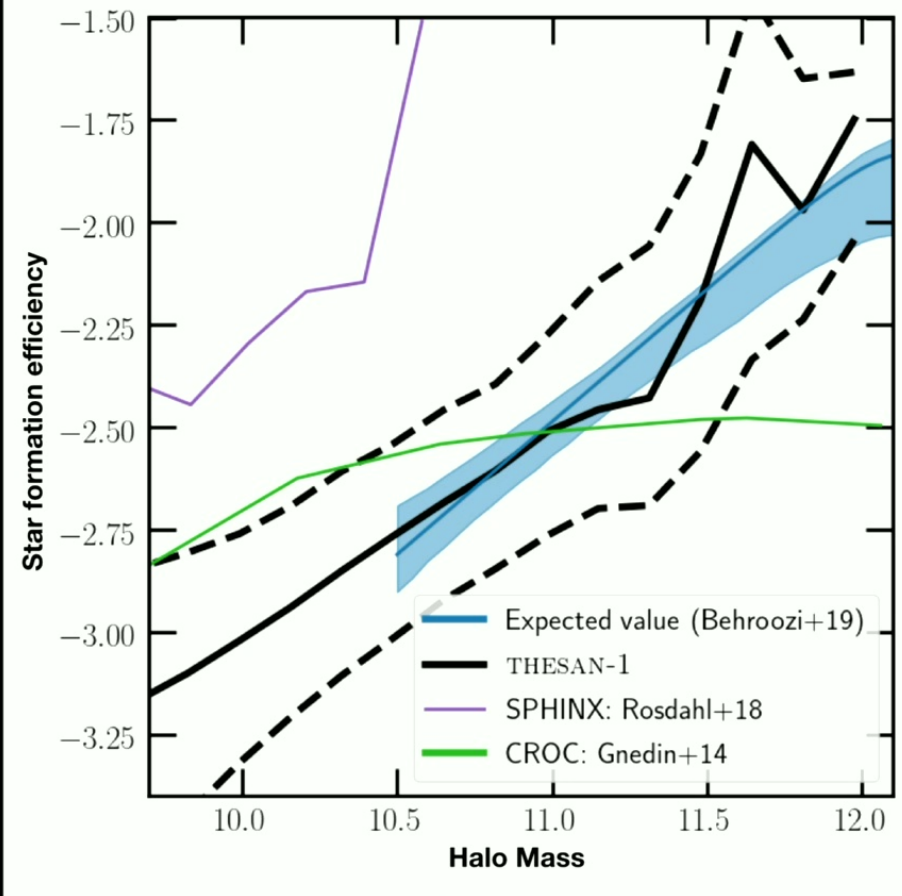
- Self-shielded filaments and knots are resolved

Kannan+22a

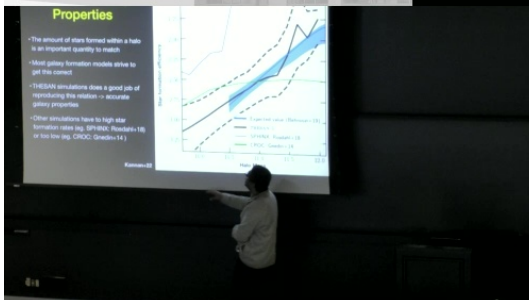


# Accurate Galaxy Properties

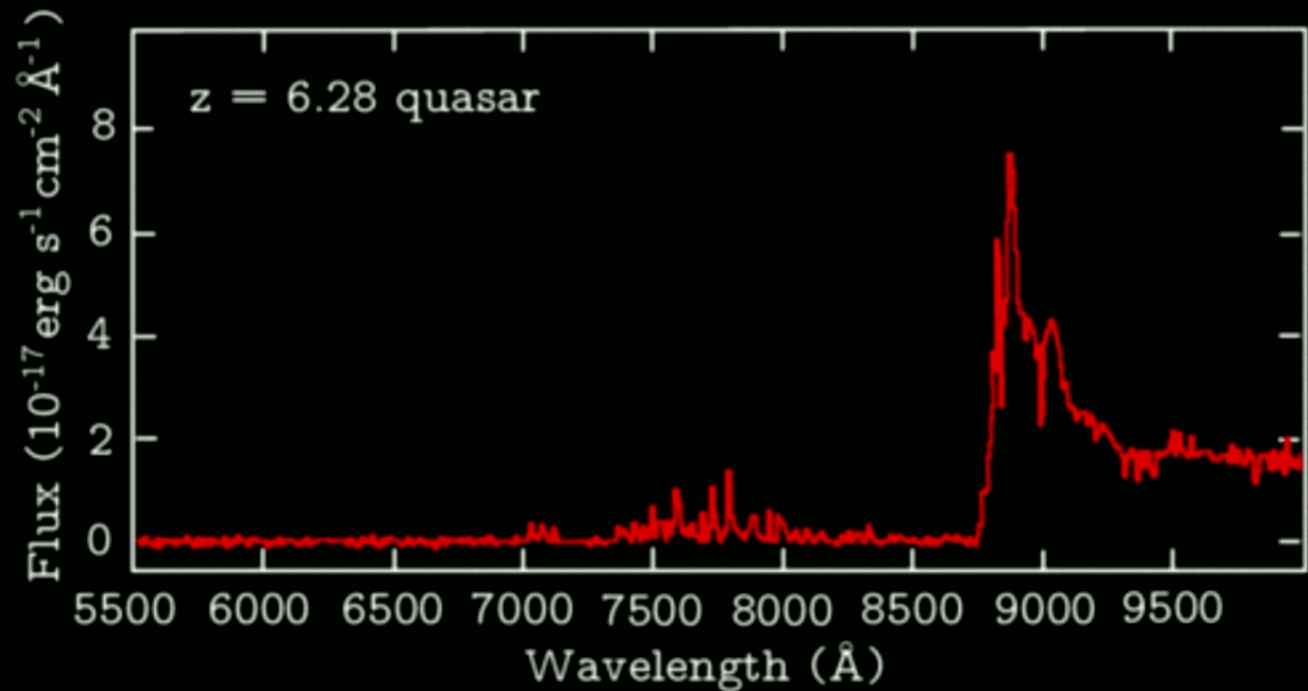
- The amount of stars formed within a halo is an important quantity to match
- Most galaxy formation models strive to get this correct
- THESAN simulations does a good job of reproducing this relation -> accurate galaxy properties
- Other simulations have to high star formation rates (eg. SPHINX: Rosdahl+18) or too low (eg. CROC: Gnedin+14 )



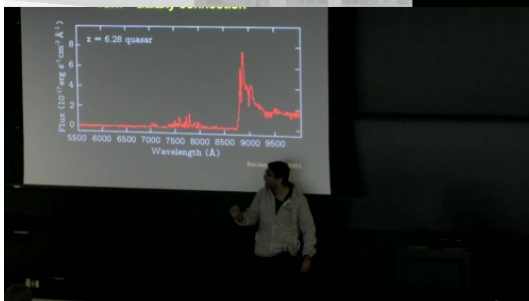
Kannan+22



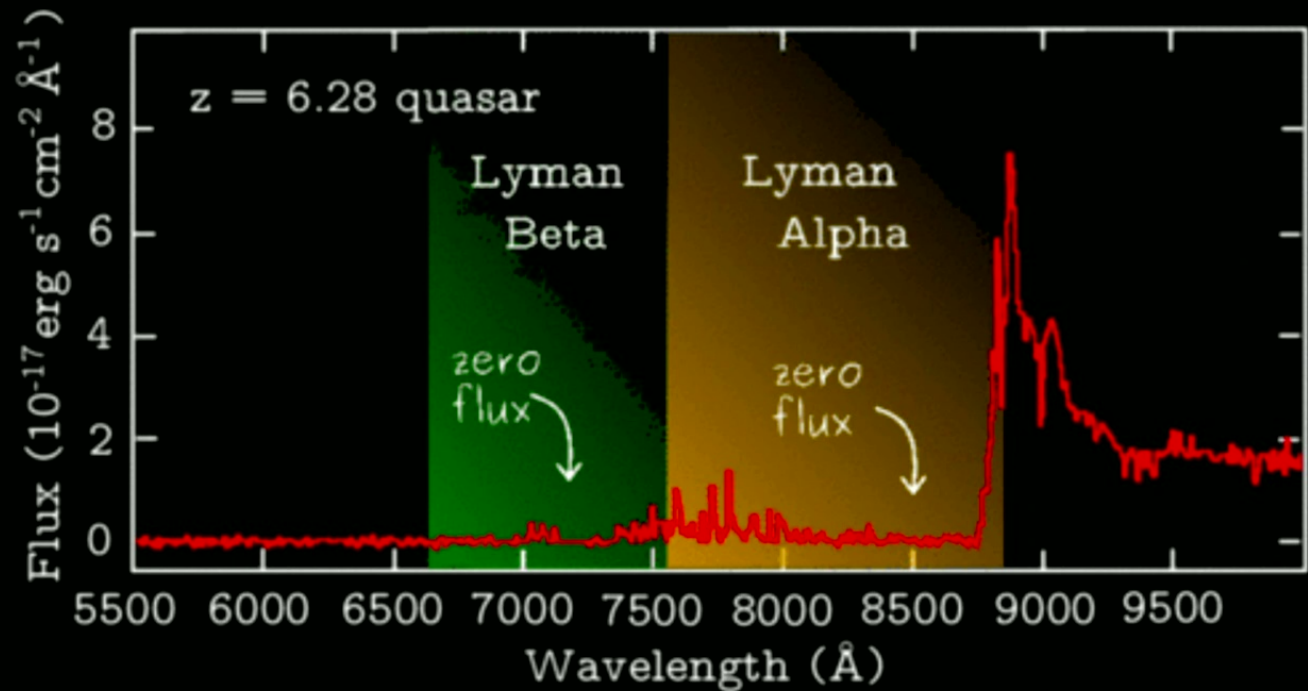
# IGM - Galaxy connection



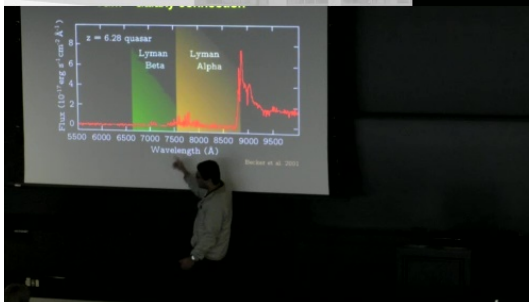
Becker et al. 2001



# IGM - Galaxy connection

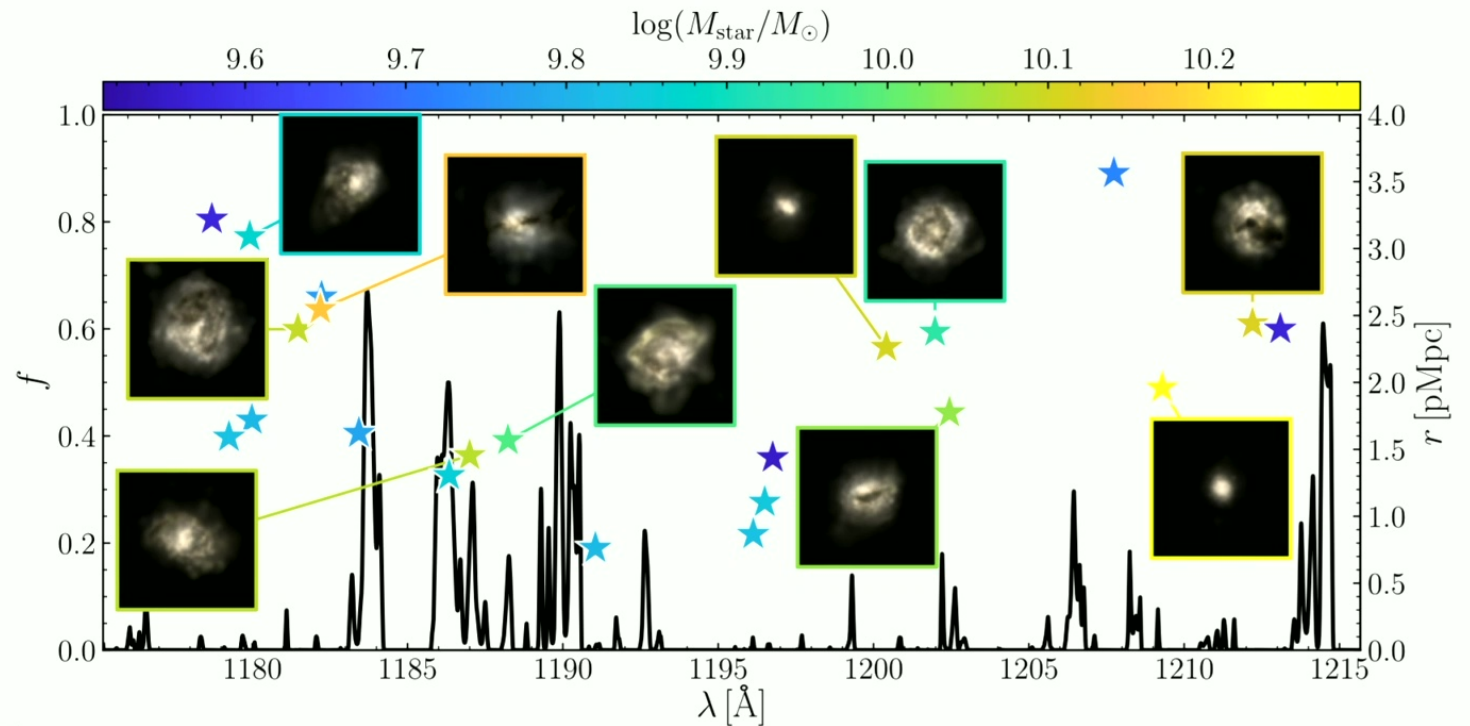


Becker et al. 2001





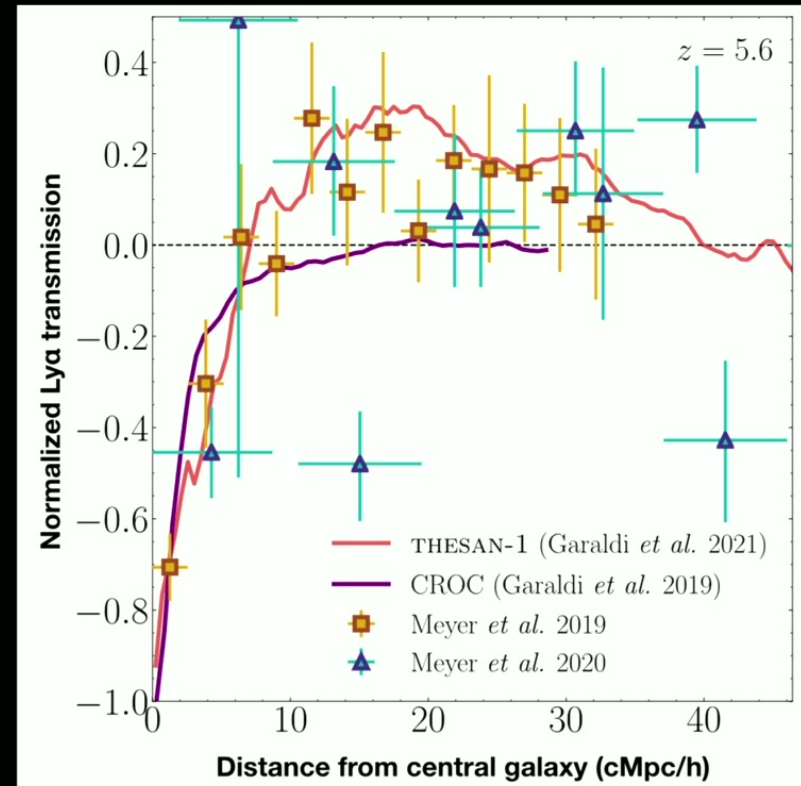
# IGM - Galaxy connection



Garaldi, Kannan+22

# IGM - Galaxy connection

- The normalized transmission flux of the Ly $\alpha$  line around galaxies is an important observable
- Previous generation of simulations not able to match the increase in transmission around galaxies
- THESAN matches the observational points offering a path to study physical reason to study enhanced emission around galaxies



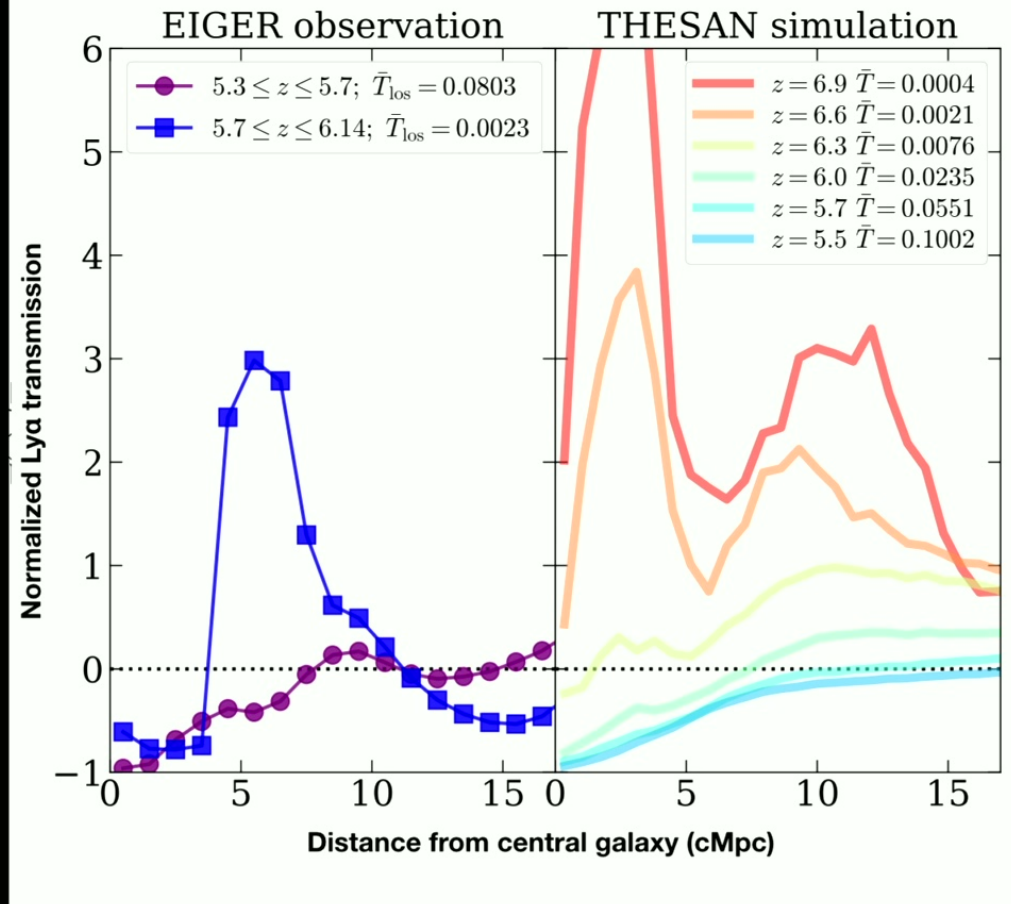
Garaldi, Kannan+22



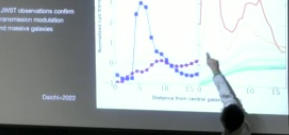
# IGM - Galaxy connection

- New JWST observations confirm this transmission modulation around massive galaxies

Daichi+2022



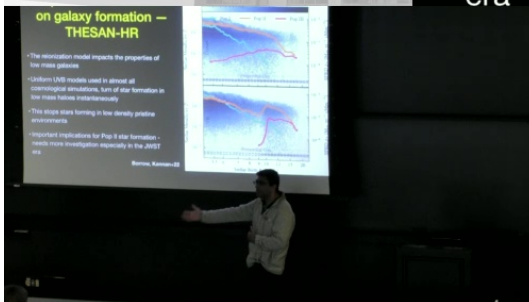
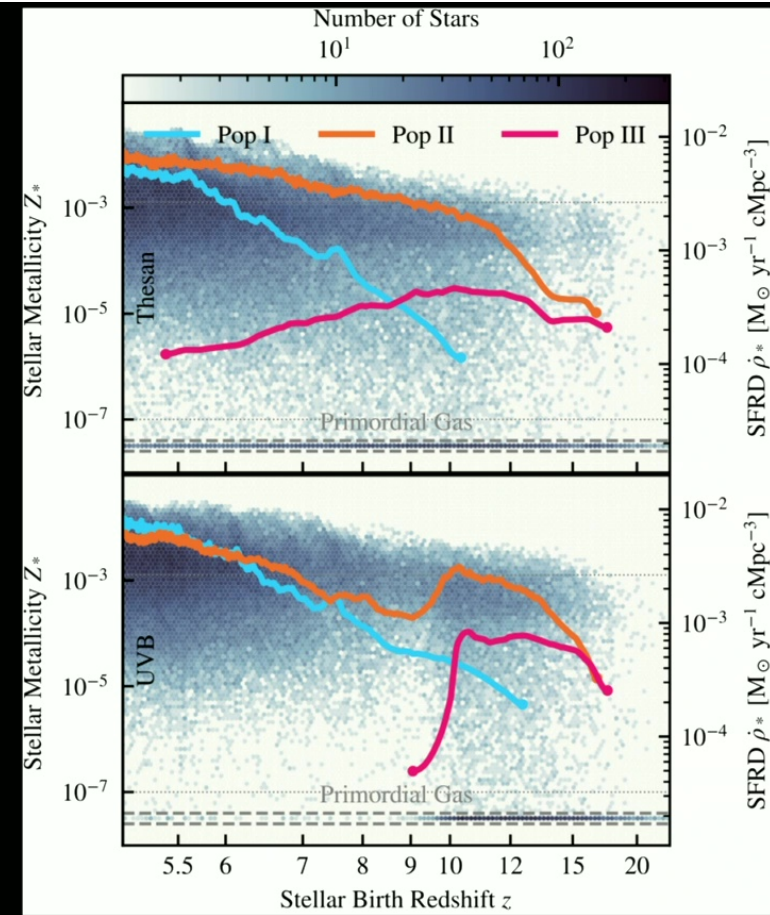
IGM - Galaxy connection



# Impact of Reionization on galaxy formation — THESAN-HR

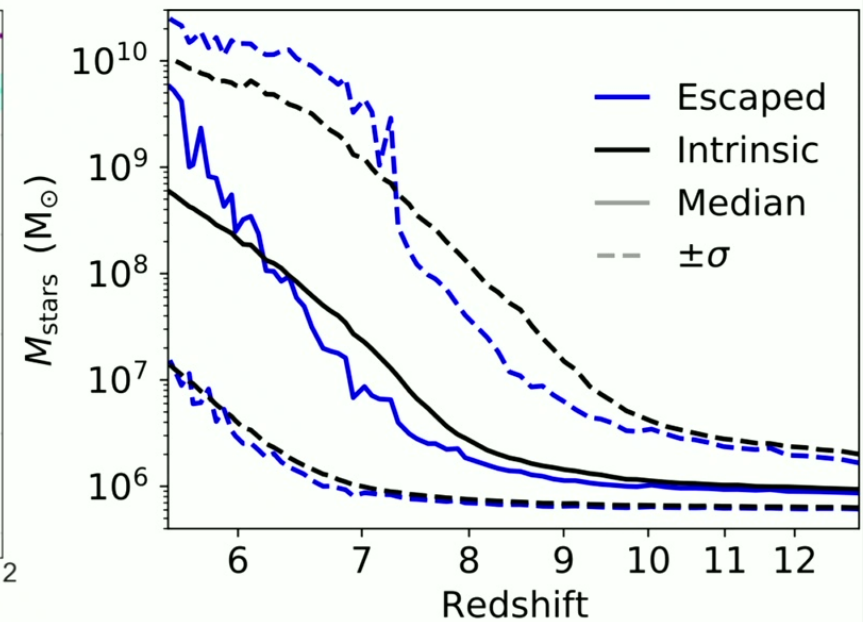
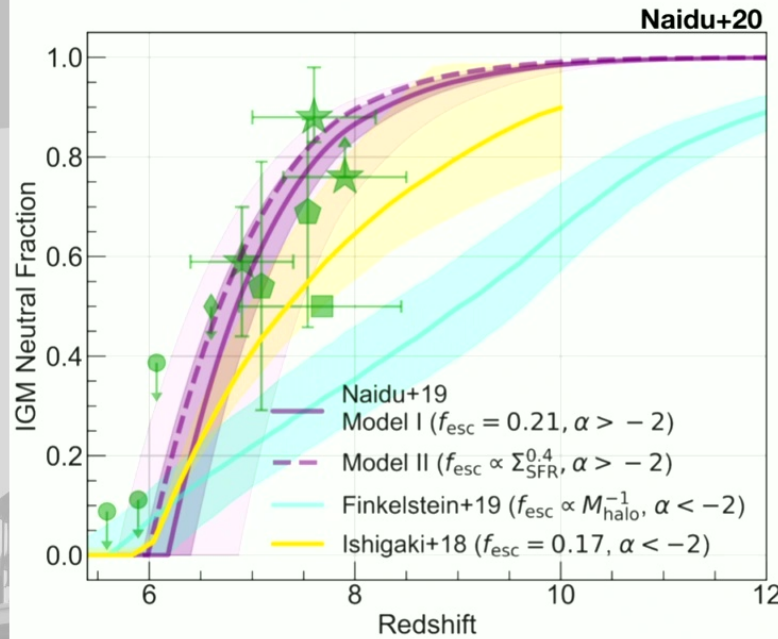
- The reionization model impacts the properties of low mass galaxies
- Uniform UVB models used in almost all cosmological simulations, turn of star formation in low mass haloes instantaneously
- This stops stars forming in low density pristine environments
- Important implications for Pop II star formation - needs more investigation especially in the JWST era

Borrow, Kannan+22





# Escape fractions from Reionization-era galaxies



• Reionization driven by high-mass or low mass galaxies?

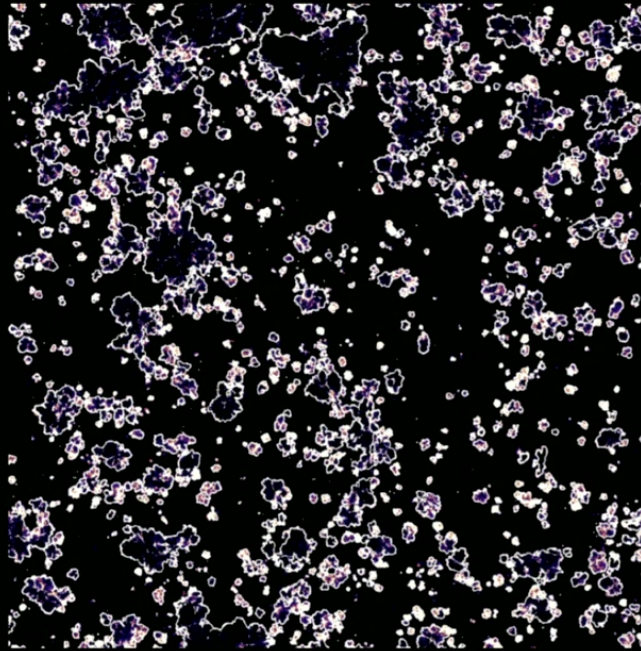
Yeh, Smith, Kannan+22

Low mass galaxies dominates at high-z and high mass galaxies at low-z

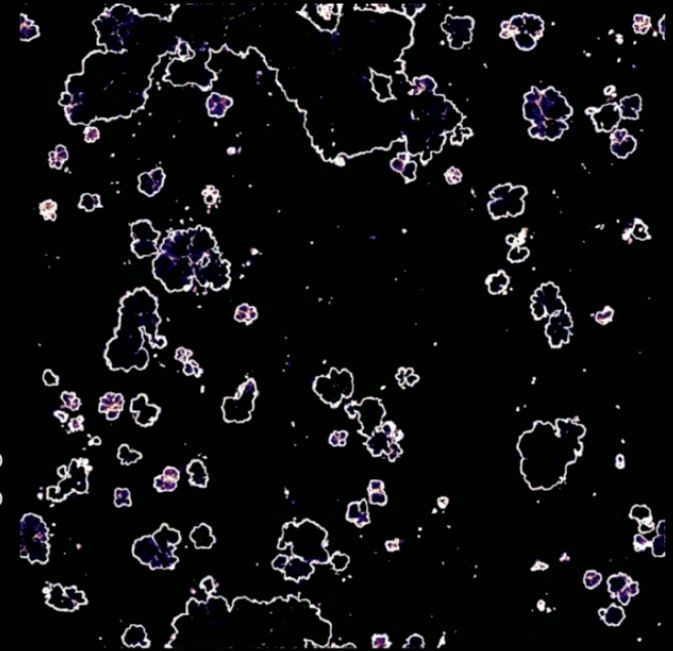


# Bubble Size Statistics

Small galaxies dominate reionization

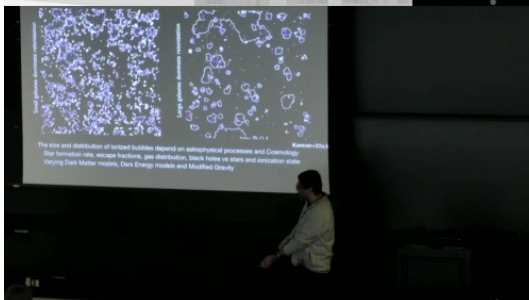


Large galaxies dominate reionization

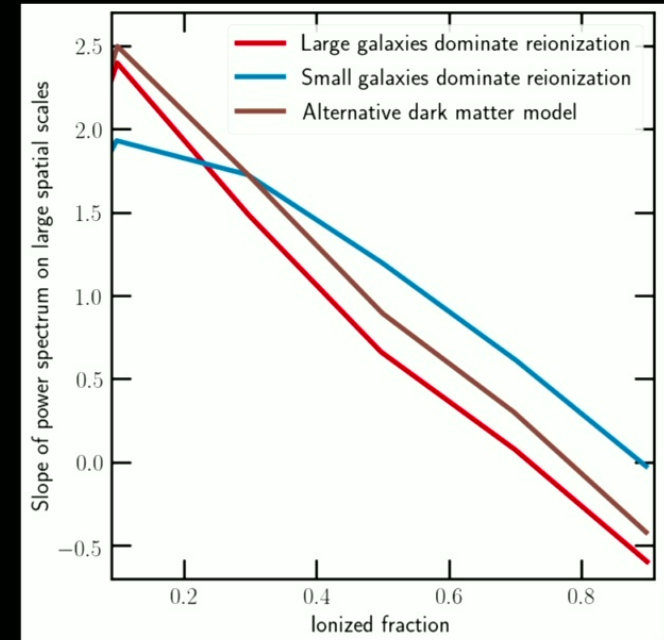
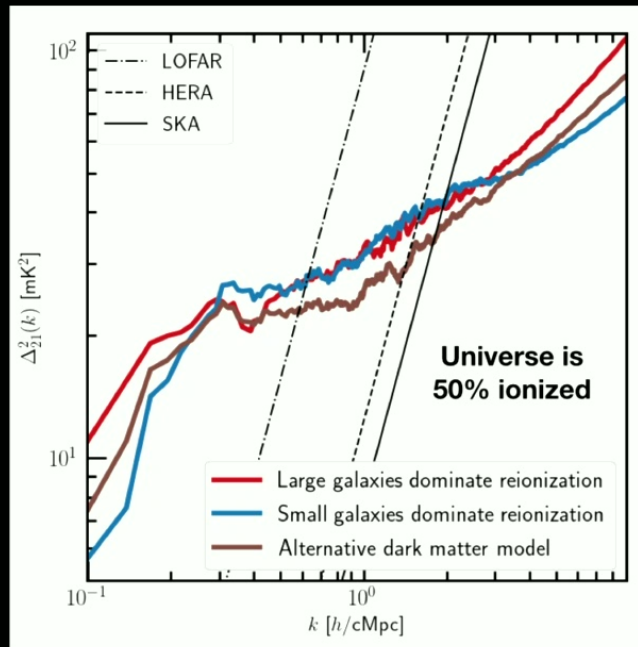


Kannan+22a,b

- The size and distribution of ionized bubbles depend on astrophysical processes and Cosmology
- Star formation rate, escape fractions, gas distribution, black holes vs stars and ionization state
- Varying Dark Matter models, Dark Energy models and Modified Gravity

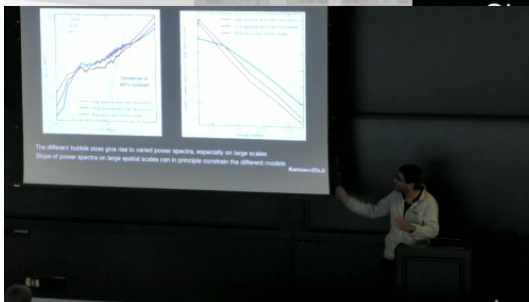


# Bubble Size Statistics



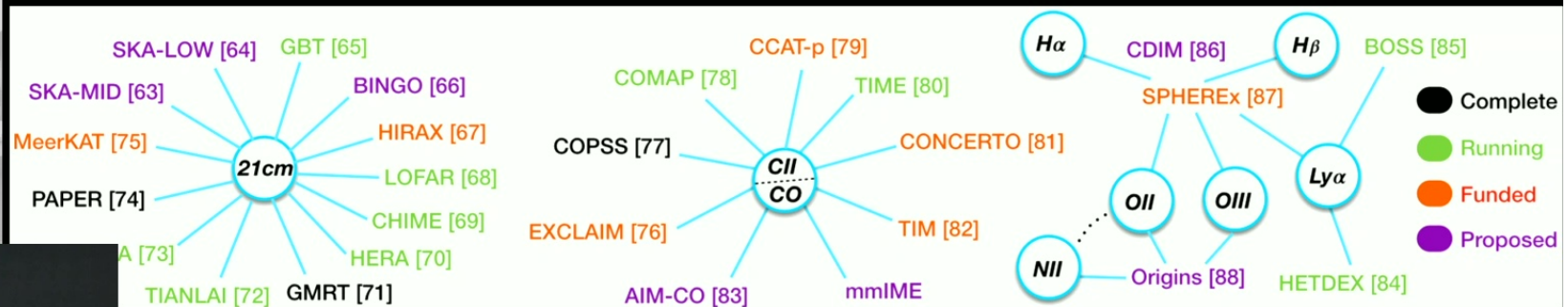
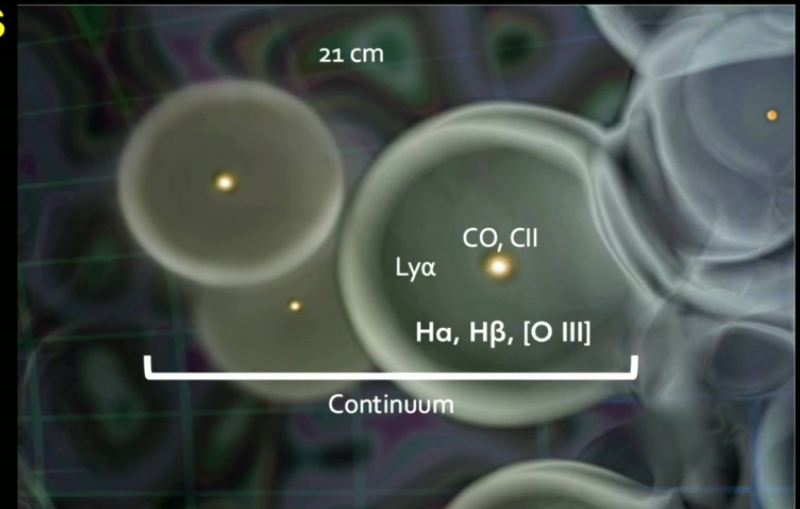
- The different bubble sizes give rise to varied power spectra, especially on large scales
- Slope of power spectra on large spatial scales can in principle constrain the different models

Kannan+22a,b



# LIM of Nebular emission lines

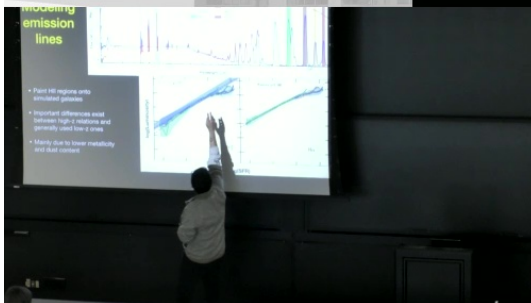
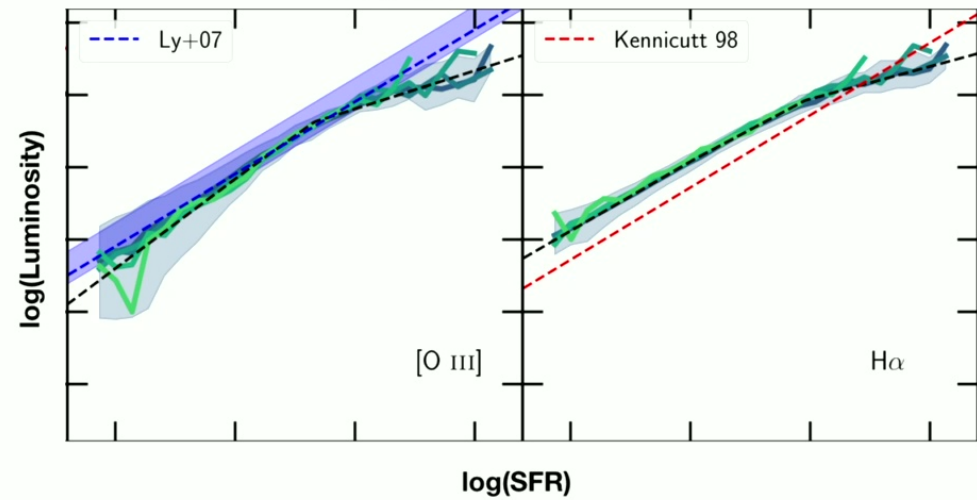
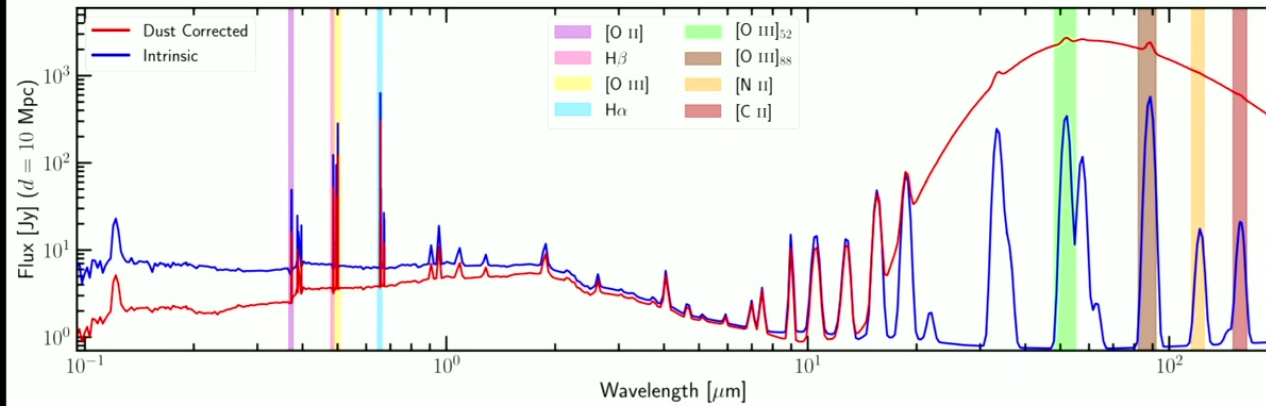
- Similar to 21cm intensity mapping
- Mapping individual emission lines mainly arising from HII regions
- 21 cm contains information about the reionization process while nebular LIM traces the sources responsible for it





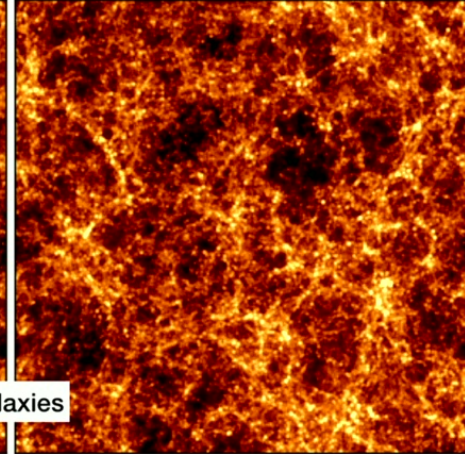
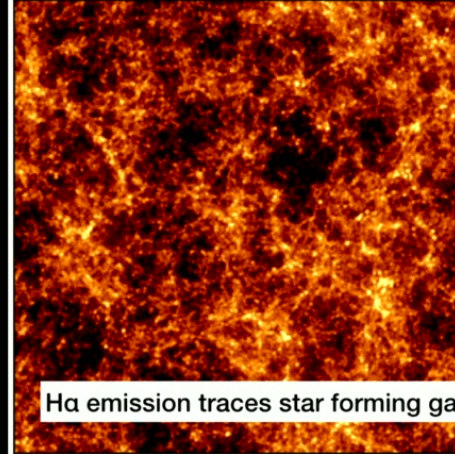
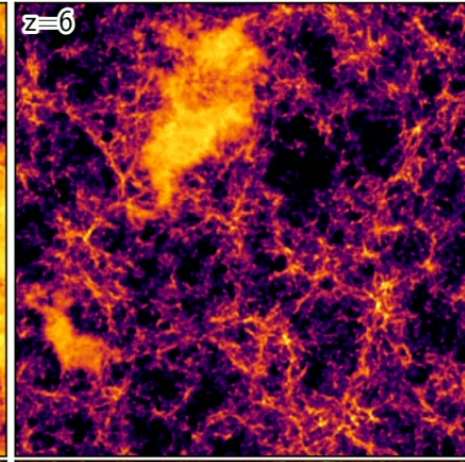
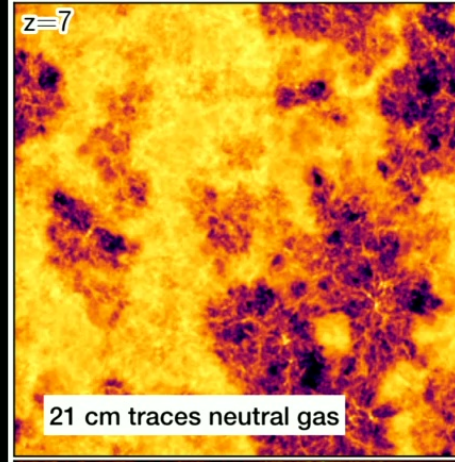
# Modeling emission lines

- Paint HII regions onto simulated galaxies
- Important differences exist between high-z relations and generally used low-z ones
- Mainly due to lower metallicity and dust content

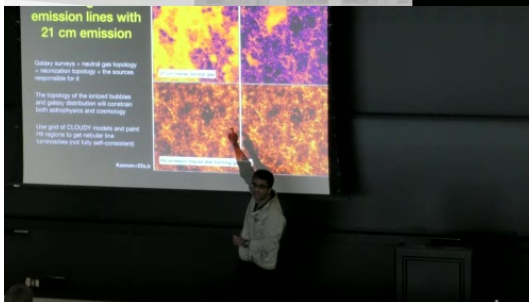


# Combining nebular emission lines with 21 cm emission

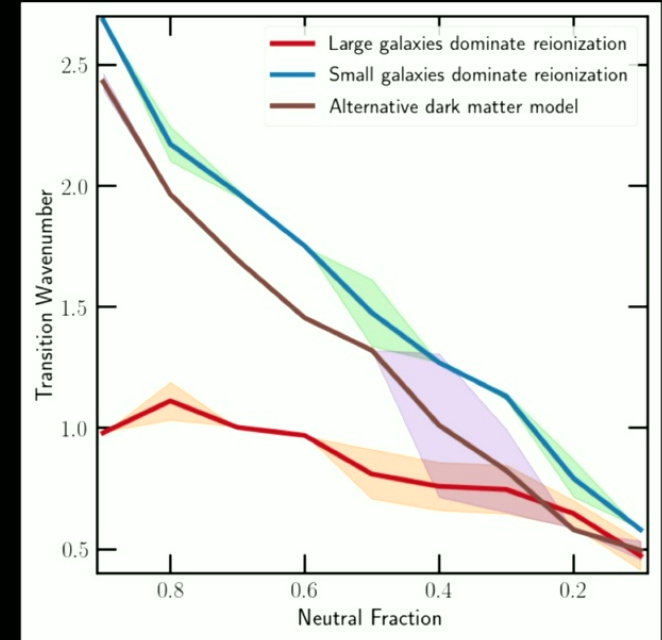
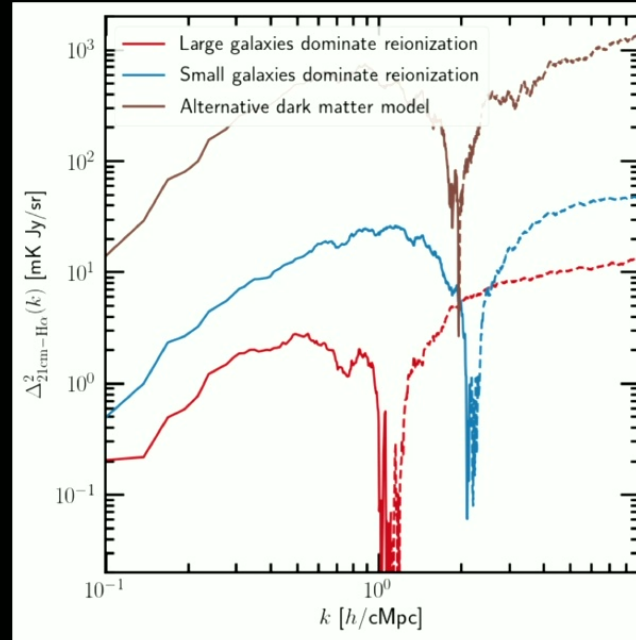
- Galaxy surveys + neutral gas topology = reionization topology + the sources responsible for it
- The topology of the ionized bubbles and galaxy distribution will constrain both astrophysics and cosmology
- Use grid of CLOUDY models and paint HII regions to get nebular line luminosities (not fully self-consistent)



Kannan+22a,b



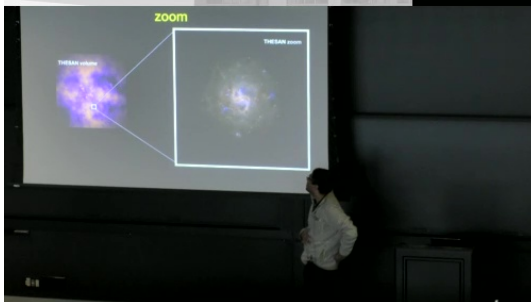
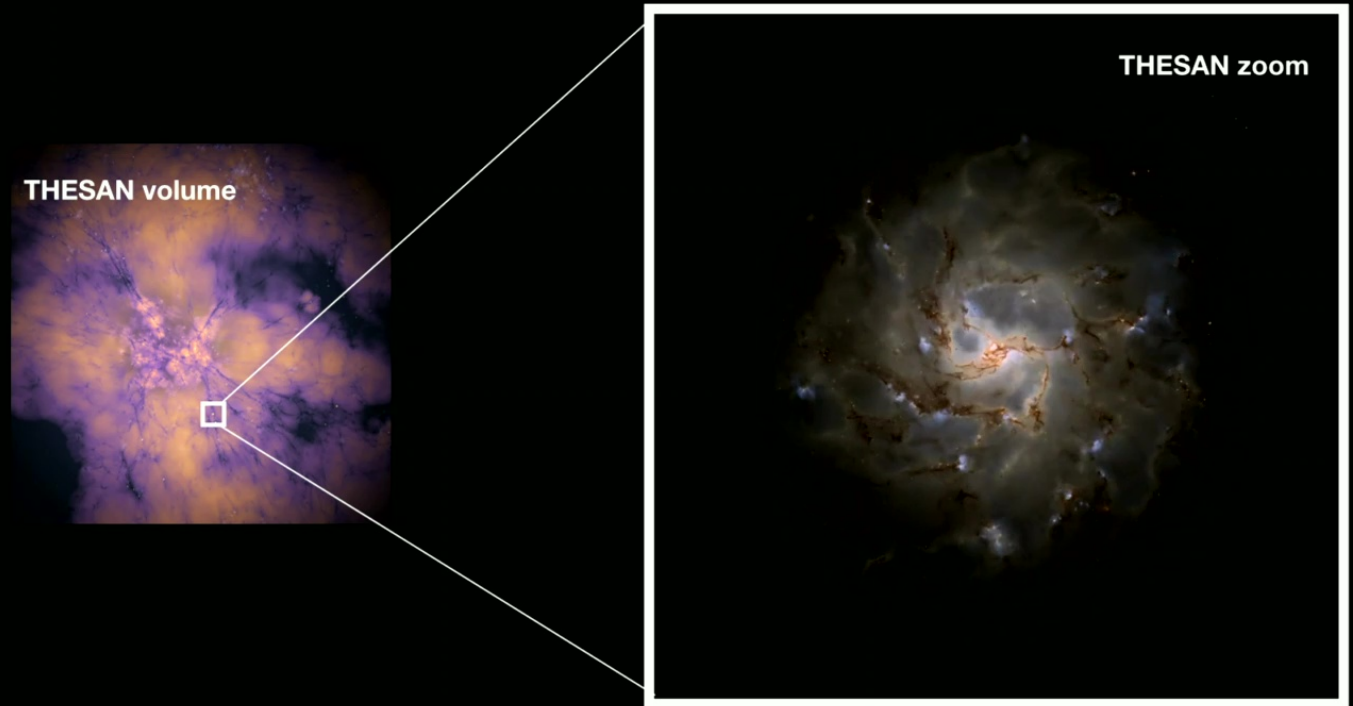
# Nebular emission lines + 21 cm



- Cross - correlation between nebular emission line and 21 cm maps inform us about the reionization process
  - Solid curve - negative correlation
  - Dashed curve - positive correlation
- transition wavenumber helps constrain galaxy properties and underlying cosmology

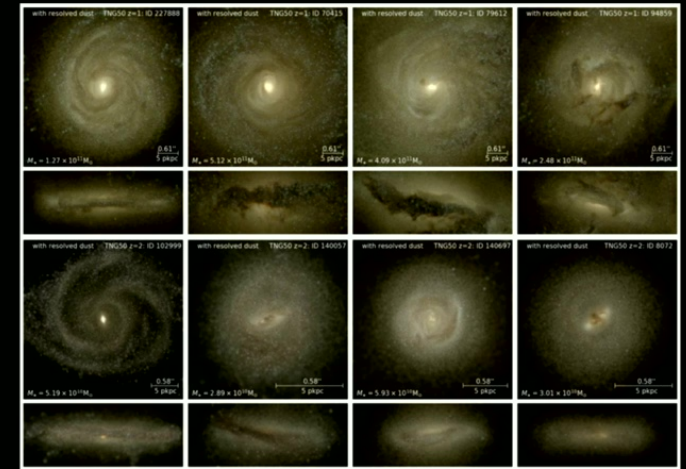
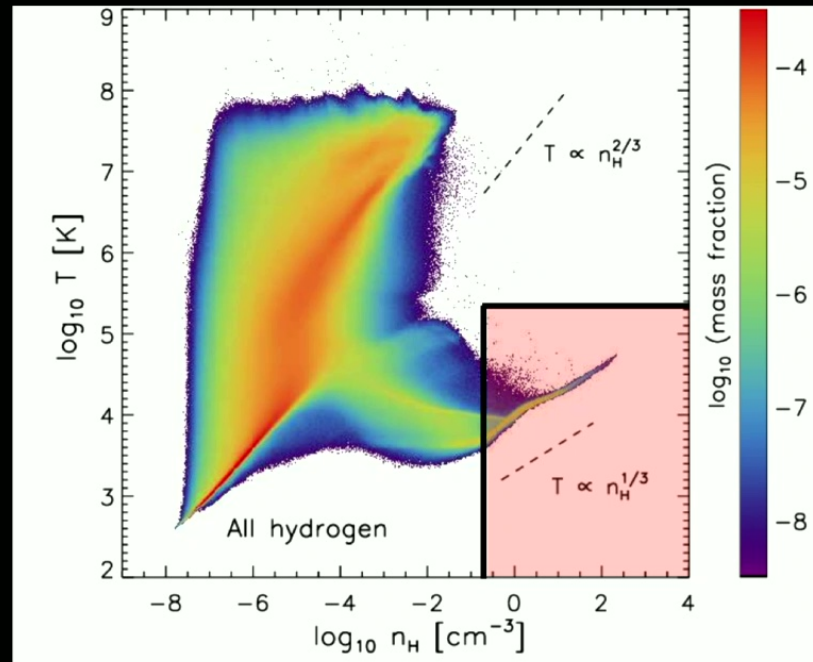
Kannan+22a,b

# Improvements to the THESAN model - THESAN zoom



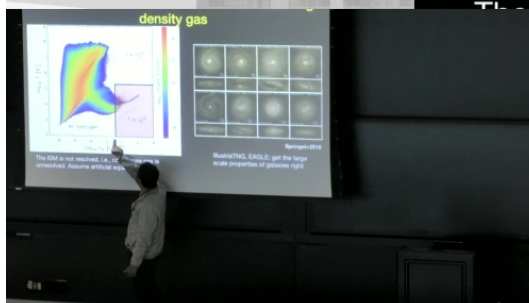


# Large volume simulations - unable to model high density gas



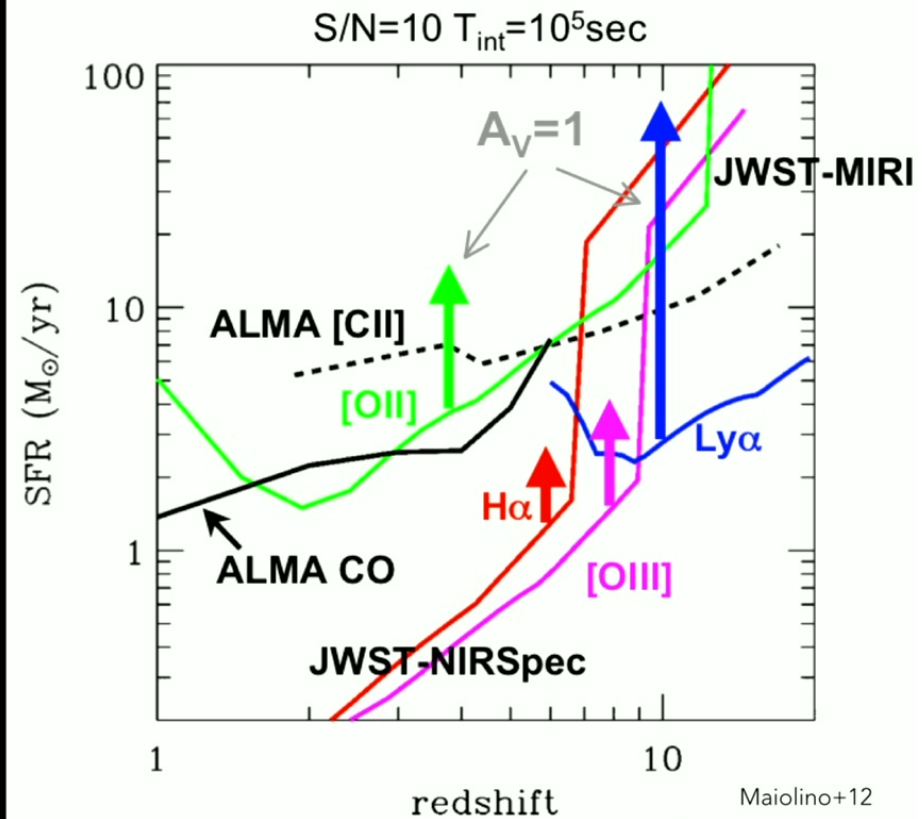
Springel+2018

IllustrisTNG, EAGLE: get the large scale properties of galaxies right



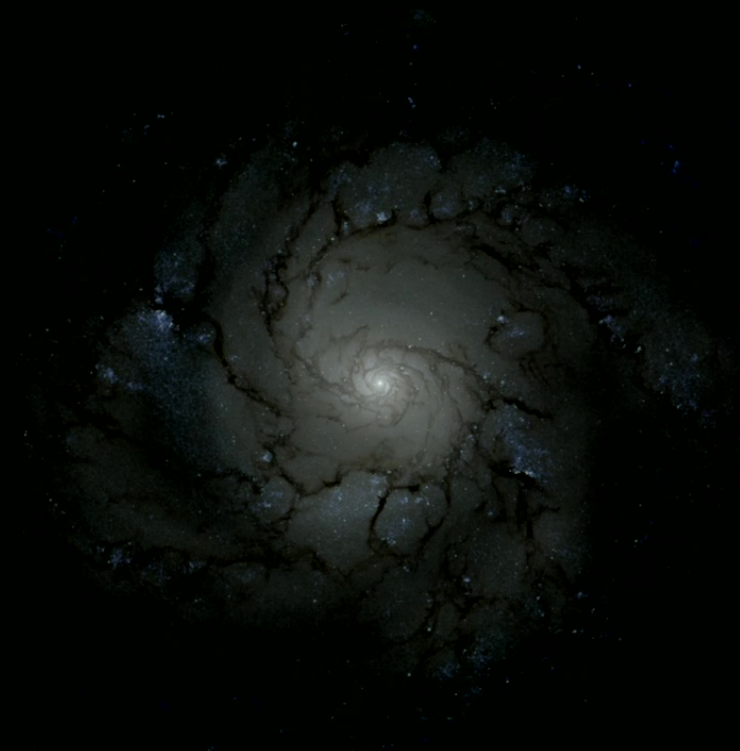
# Need to improve the state-of-the-art

- The emission lines depend on the local radiation properties in addition to density, metallicity and temperature
- JWST detects a variety of rest frame optical lines
- ALMA detects the cold phase of the ISM
- Most of these lines arise from dense ionized gas in the ISM of galaxies, making it extremely important to model this phase accurately in simulations



# Multi-phase ISM model -SMUGGLE

- Similar to FIRE models
- Multiphase ISM model
- Dense gas can cool to 10 K using fitting functions
- Sub-grid prescriptions for SNe and stellar winds
- Approximate model for radiation fields
- Lacks dust modelling
- Important processes that impact the dense ISM gas is still modeled in an approximate manner

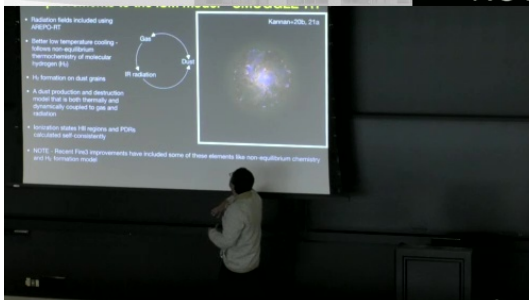
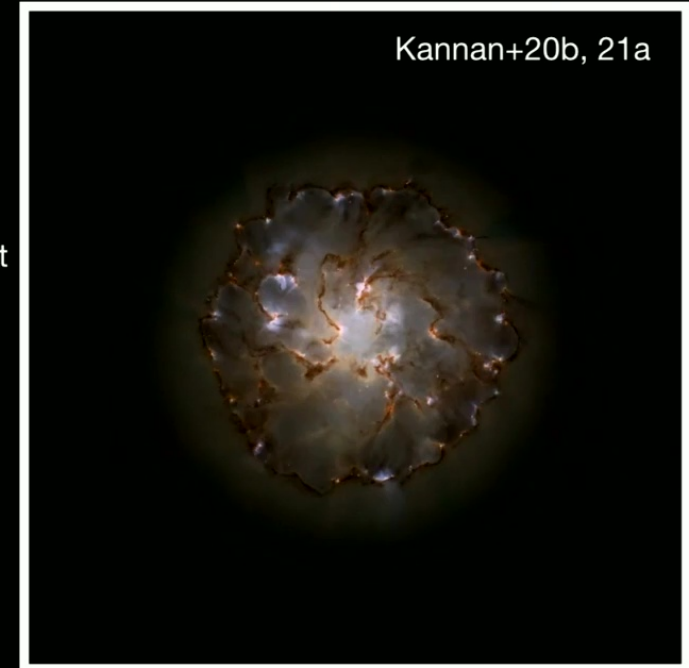
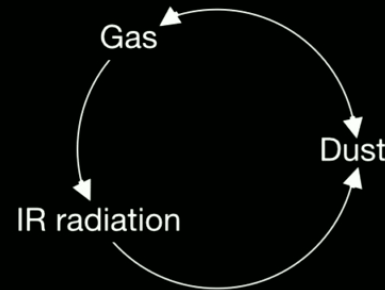


Marinacci+19



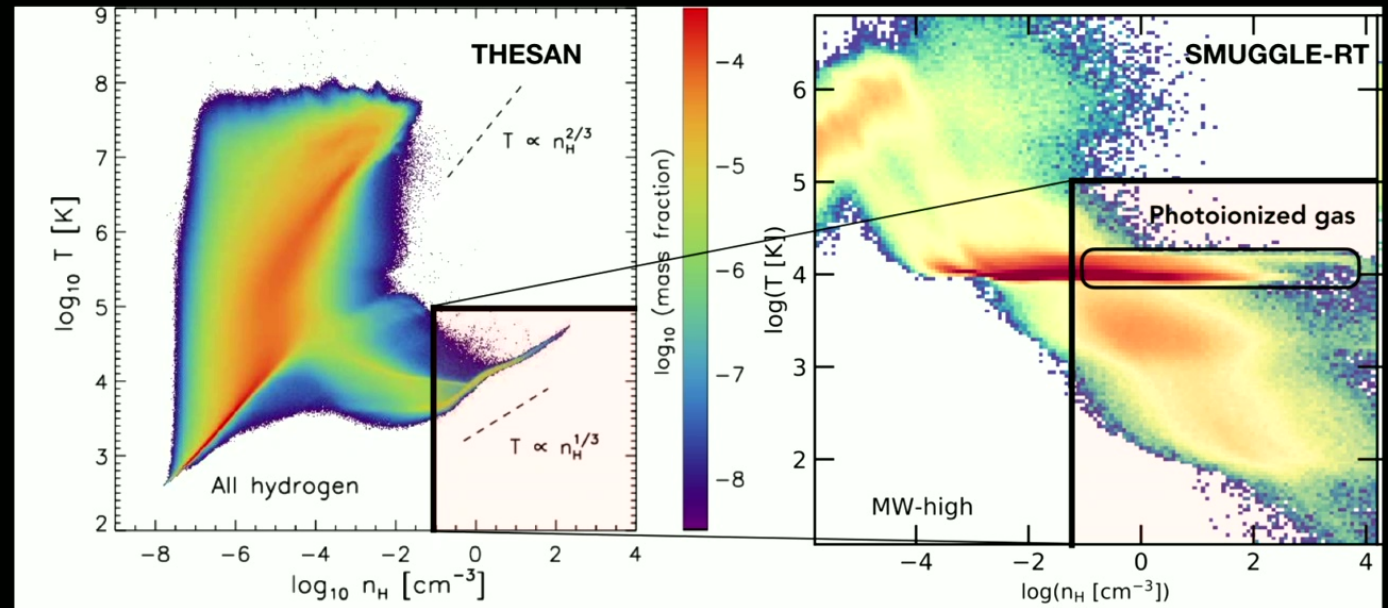
# Improvements to the ISM model - SMUGGLE-RT

- Radiation fields included using AREPO-RT
- Better low temperature cooling - follows non-equilibrium thermochemistry of molecular hydrogen ( $H_2$ )
- $H_2$  formation on dust grains
- A dust production and destruction model that is both thermally and dynamically coupled to gas and radiation
- Ionization states HII regions and PDRs calculated self-consistently
- NOTE - Recent Fire3 improvements have included some of these elements like non-equilibrium chemistry  $H_2$  formation model

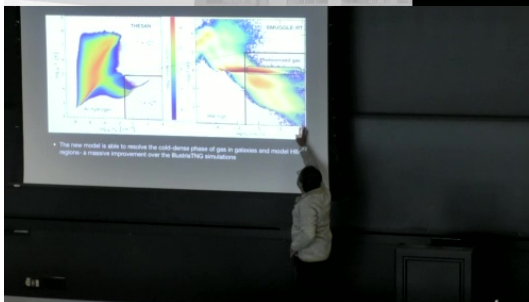




# Phase-space structure of the dense gas



- The new model is able to resolve the cold-dense phase of gas in galaxies and model HII/PDR regions- a massive improvement over the IllustrisTNG simulations

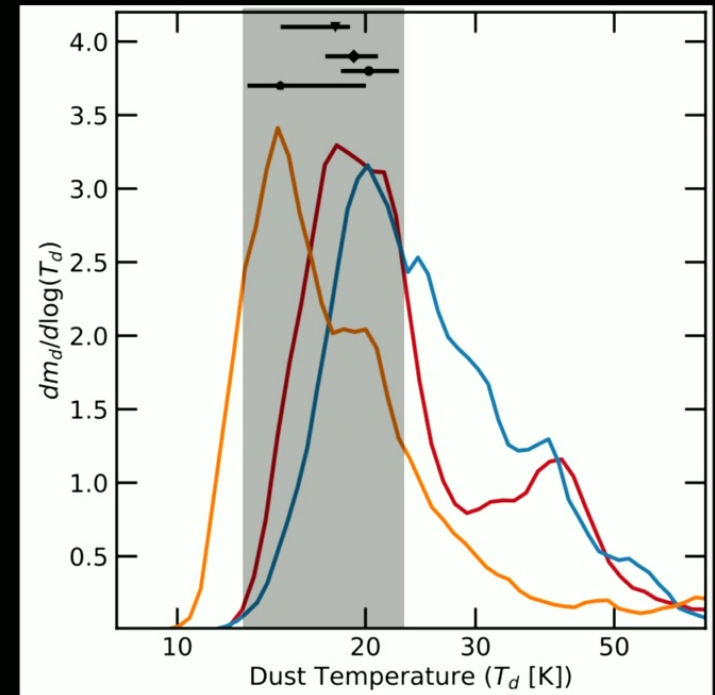
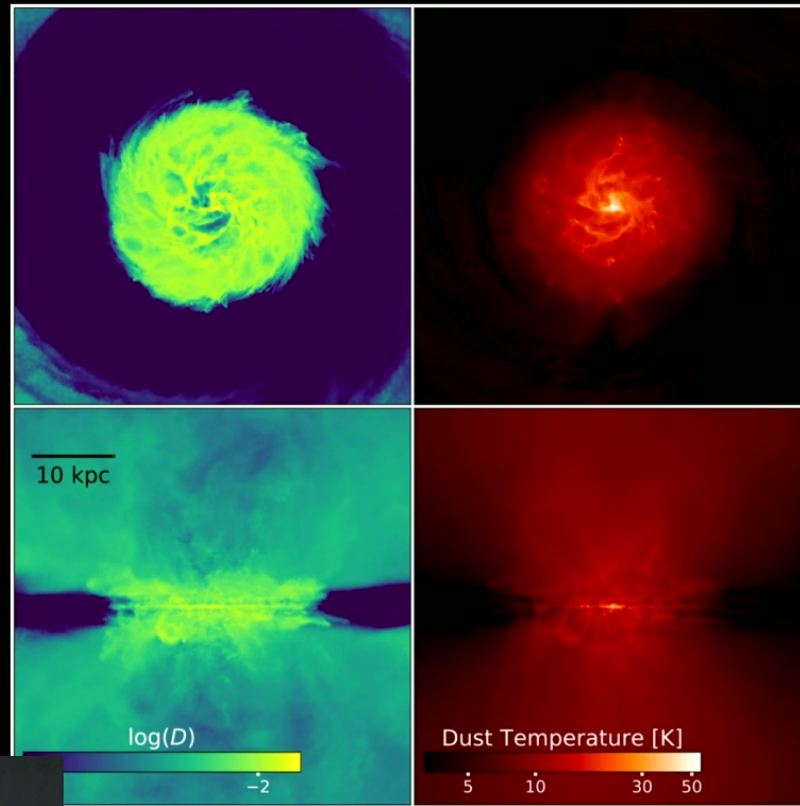


# Obscured & unobscured star formation

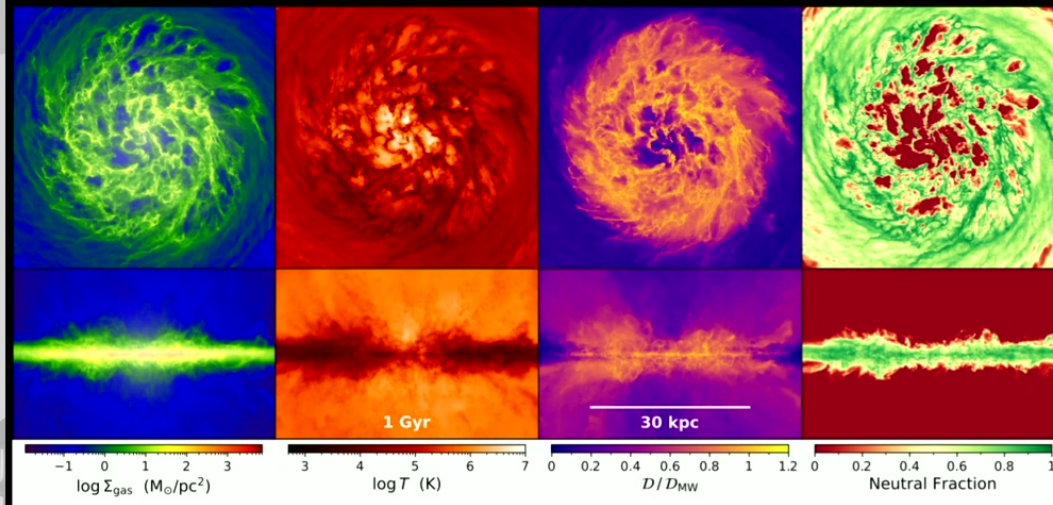
- New stars - IR bright
- Becomes UV bright as the birth cloud is disrupted



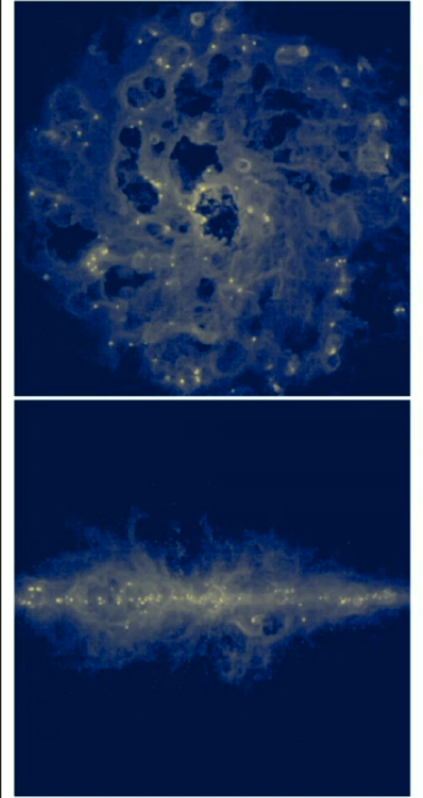
# Dust Properties



# Emission line properties



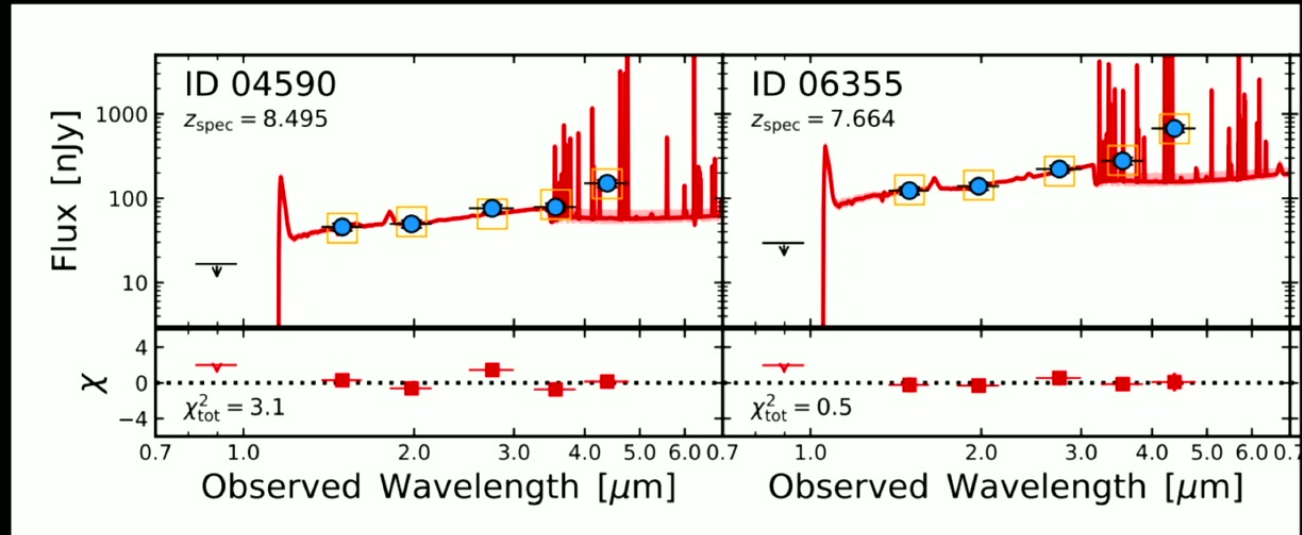
log  $\Sigma_{\text{L(H}\alpha\text{)}}$  [ $\text{erg s}^{-1} \text{pc}^{-2}$ ]



Tacchella, Smith, Kannan+22; Smith, Kannan+22

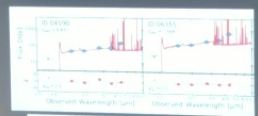


# Metal emission line predictions

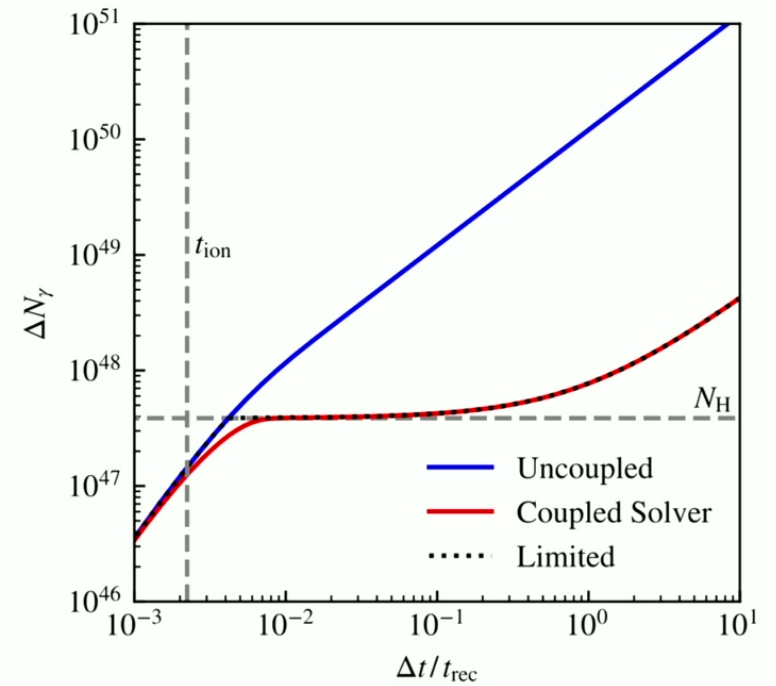
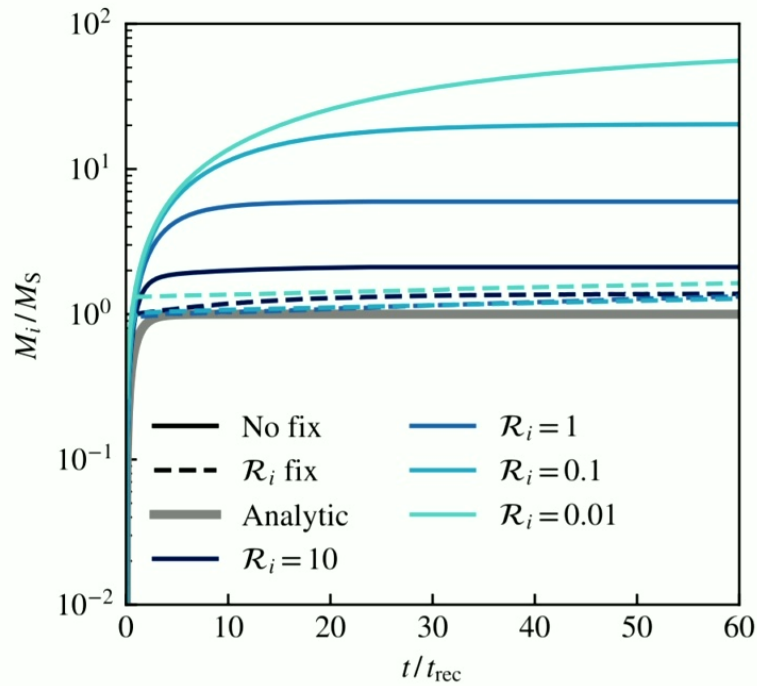


In the fitting, we mask the following emission lines: [OIII]4364, H $\delta$ , H $\zeta$ , and [NeIII]3870. We mask [OIII]4364 because we cannot reproduce very high [OIII]4364 emission line fluxes (as measured here) with our current cloudy-based modelling for the nebular emission (see next section), which includes a too narrow range in the ionization parameter. We mask H $\delta$  because this line is abnormally weak, i.e.

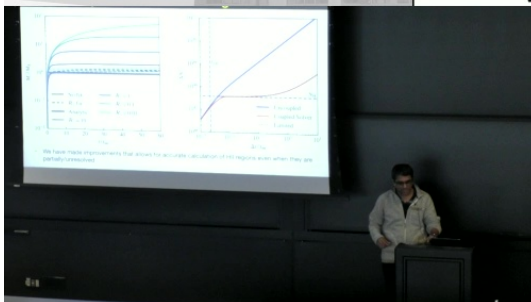
Tacchella+22 — JWST



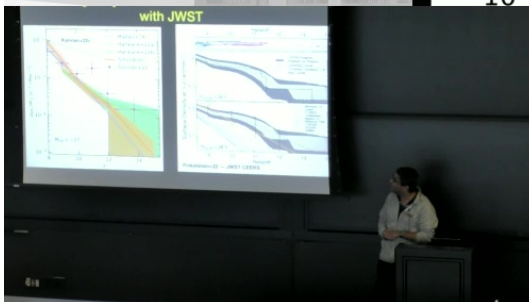
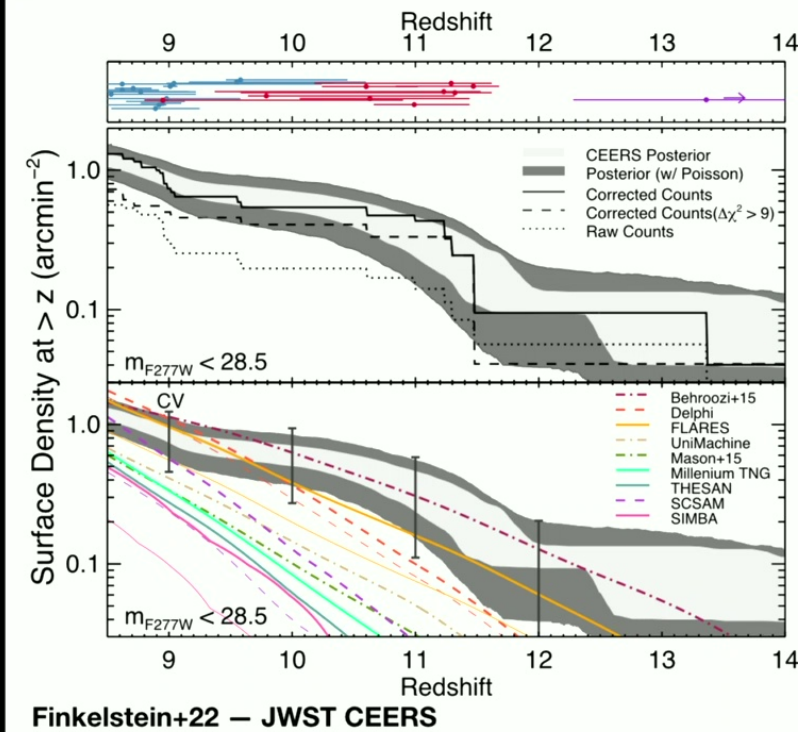
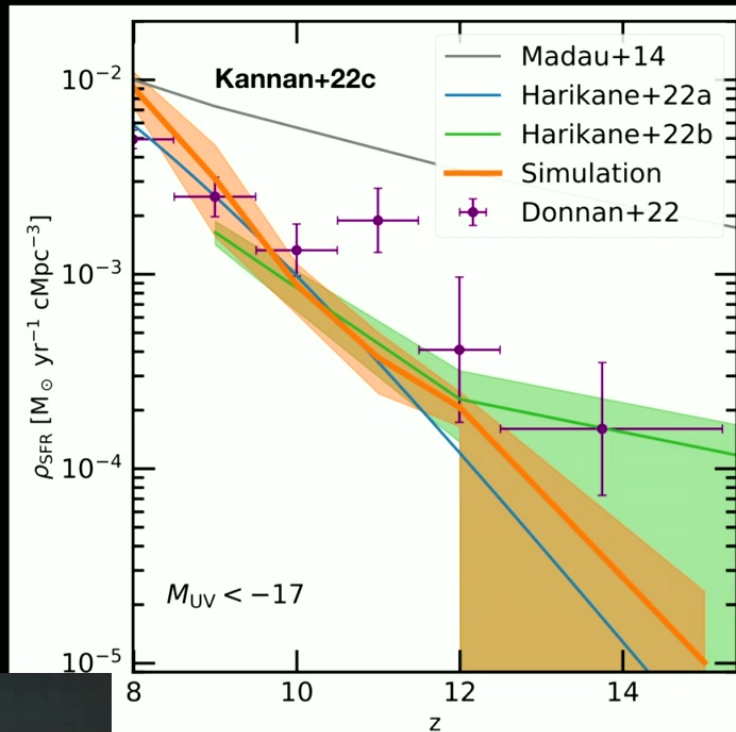
# Improvements to RHD algorithm



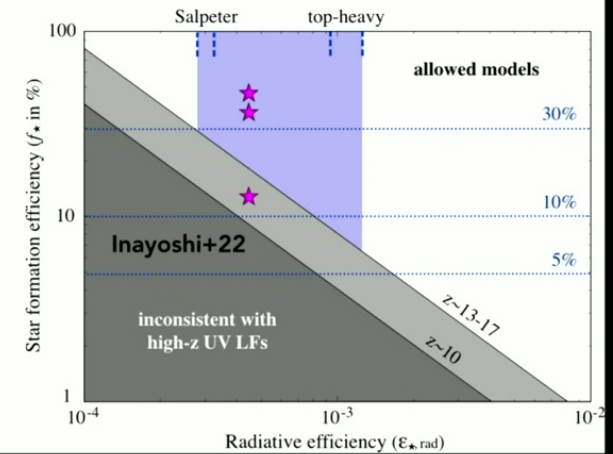
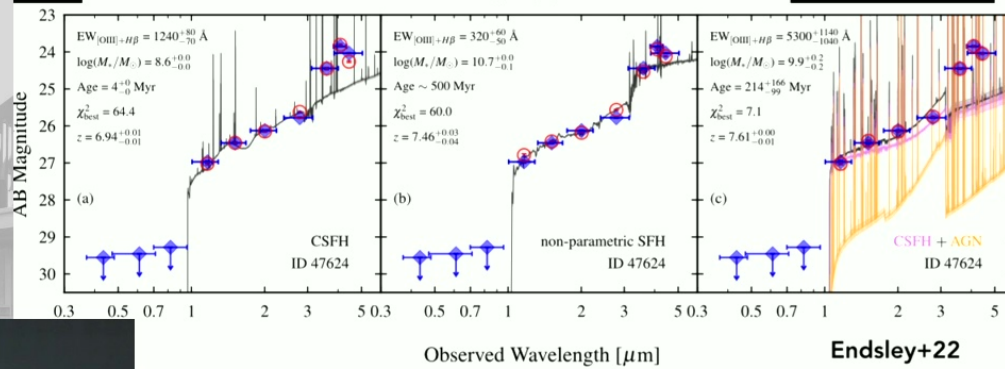
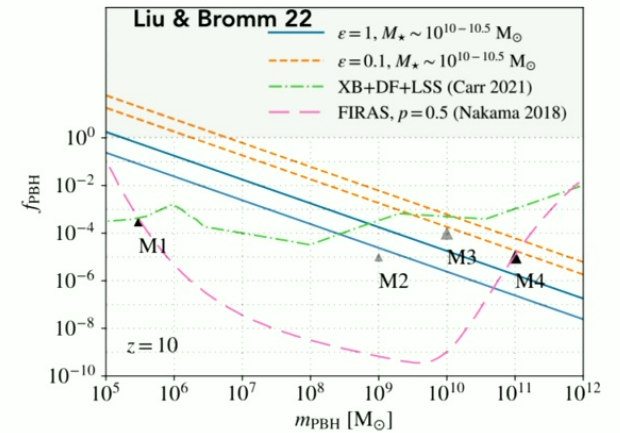
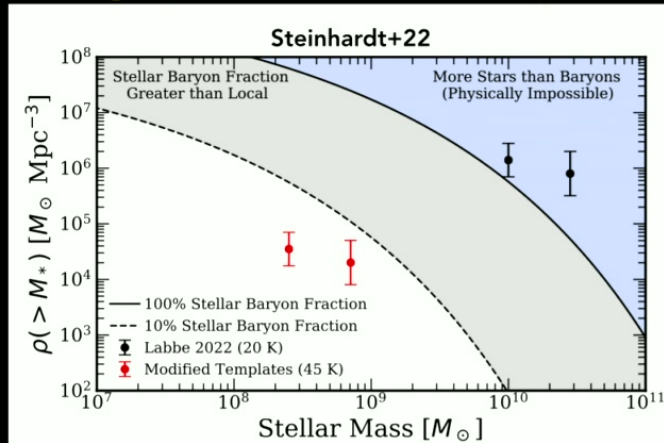
- We have made improvements that allows for accurate calculation of HII regions even when they are partially/unresolved



# Current galaxy formation models are in tension with JWST



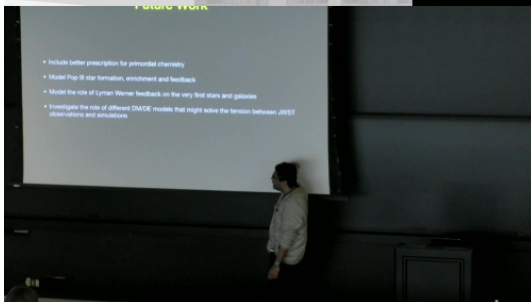
# Many plausible explanations





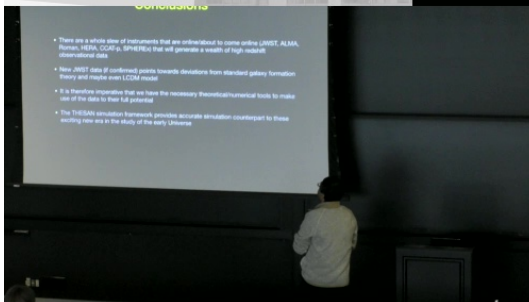
# Future Work

- Include better prescription for primordial chemistry
- Model Pop III star formation, enrichment and feedback
- Model the role of Lyman Werner feedback on the very first stars and galaxies
- Investigate the role of different DM/DE models that might solve the tension between JWST observations and simulations



# Conclusions

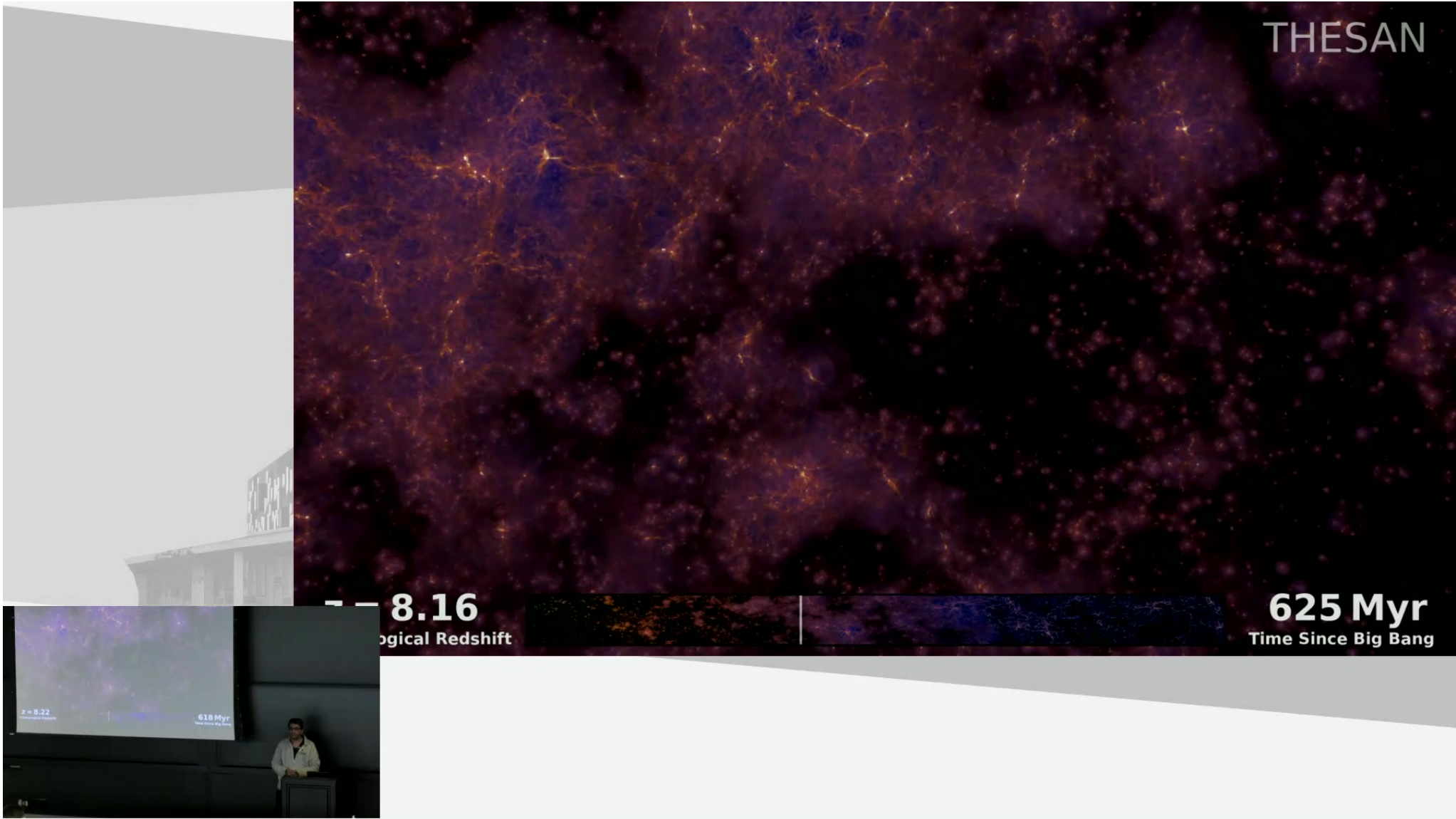
- There are a whole slew of instruments that are online/about to come online (JWST, ALMA, Roman, HERA, CCAT-p, SPHEREx) that will generate a wealth of high redshift observational data
- New JWST data (if confirmed) points towards deviations from standard galaxy formation theory and maybe even LCDM model
- It is therefore imperative that we have the necessary theoretical/numerical tools to make use of the data to their full potential
- The THESAN simulation framework provides accurate simulation counterpart to these exciting new era in the study of the early Universe



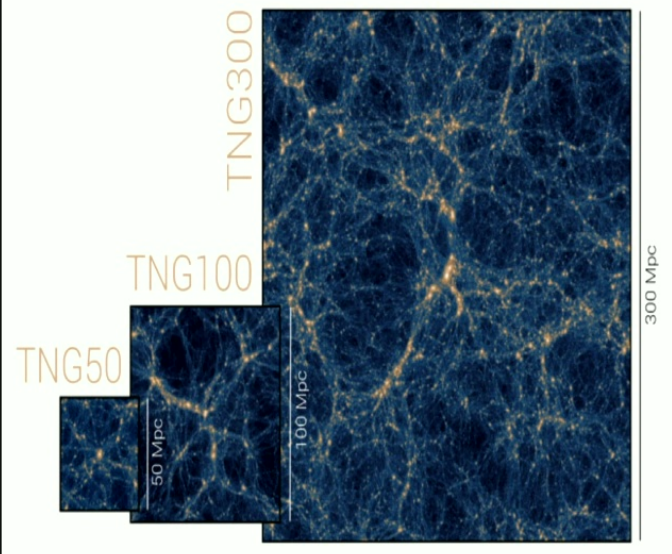








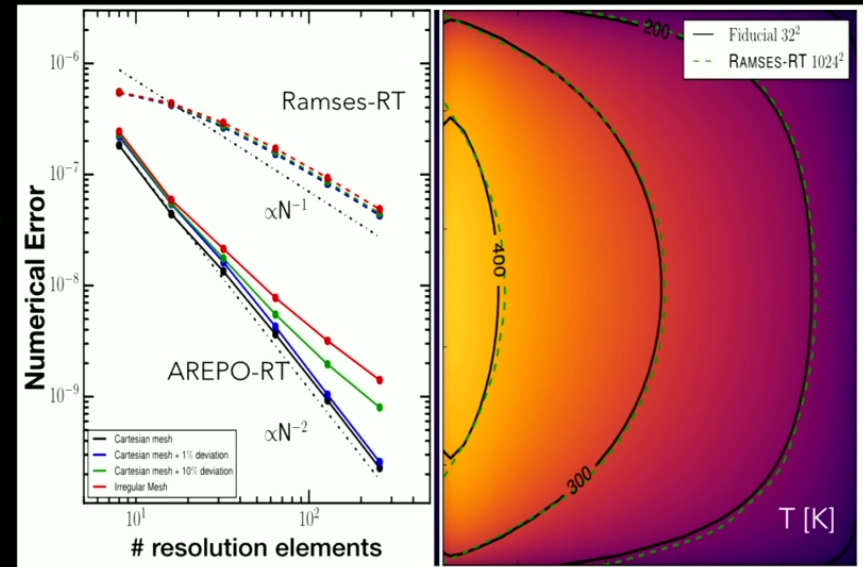
# Accurate galaxy formation model + RHD



IllustrisTNG  
(Springel+18)

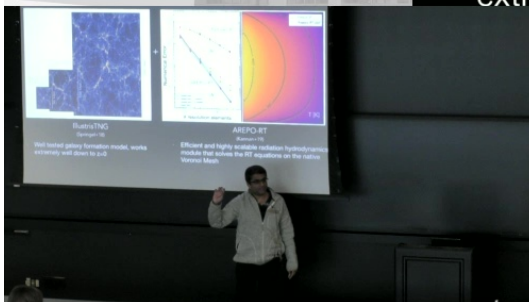
- Well tested galaxy formation model, works extremely well down to  $z=0$

+

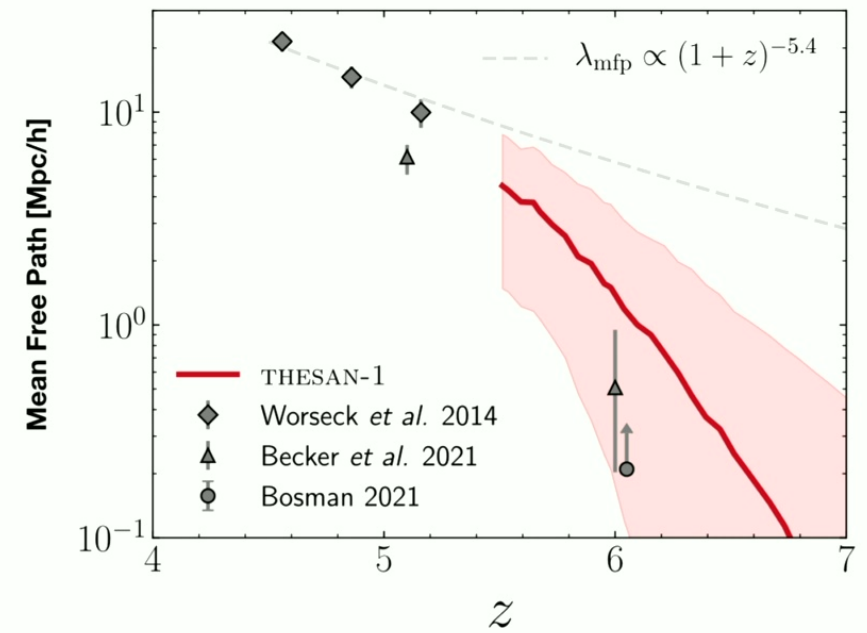
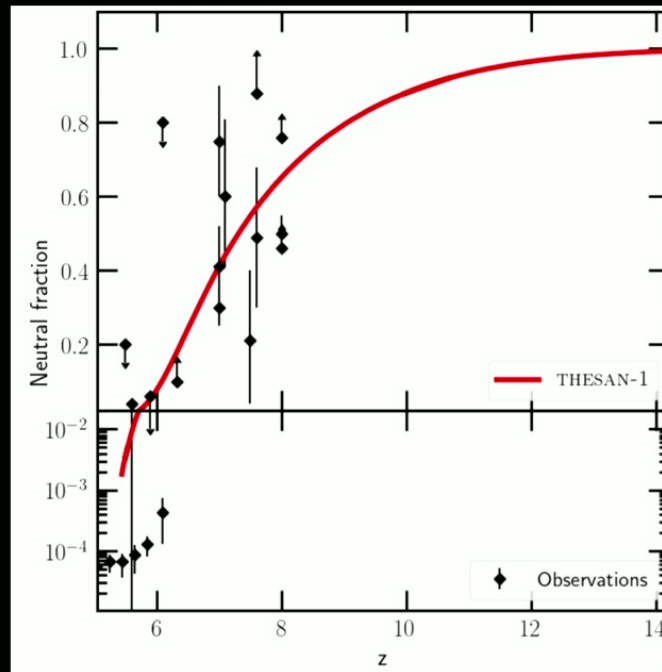


AREPO-RT  
(Kannan+19)

- Efficient and highly scalable radiation hydrodynamics module that solves the RT equations on the native Voronoi Mesh



# Accurate Reionization History



Kannan+22; Garaldi, Kannan+22

- Matches ionization history

model rapid mean free path evolution without resorting to sub-grid sink models (Cain+21, Davies+21)

