



Illustration: M. Muñoz-Echeverría

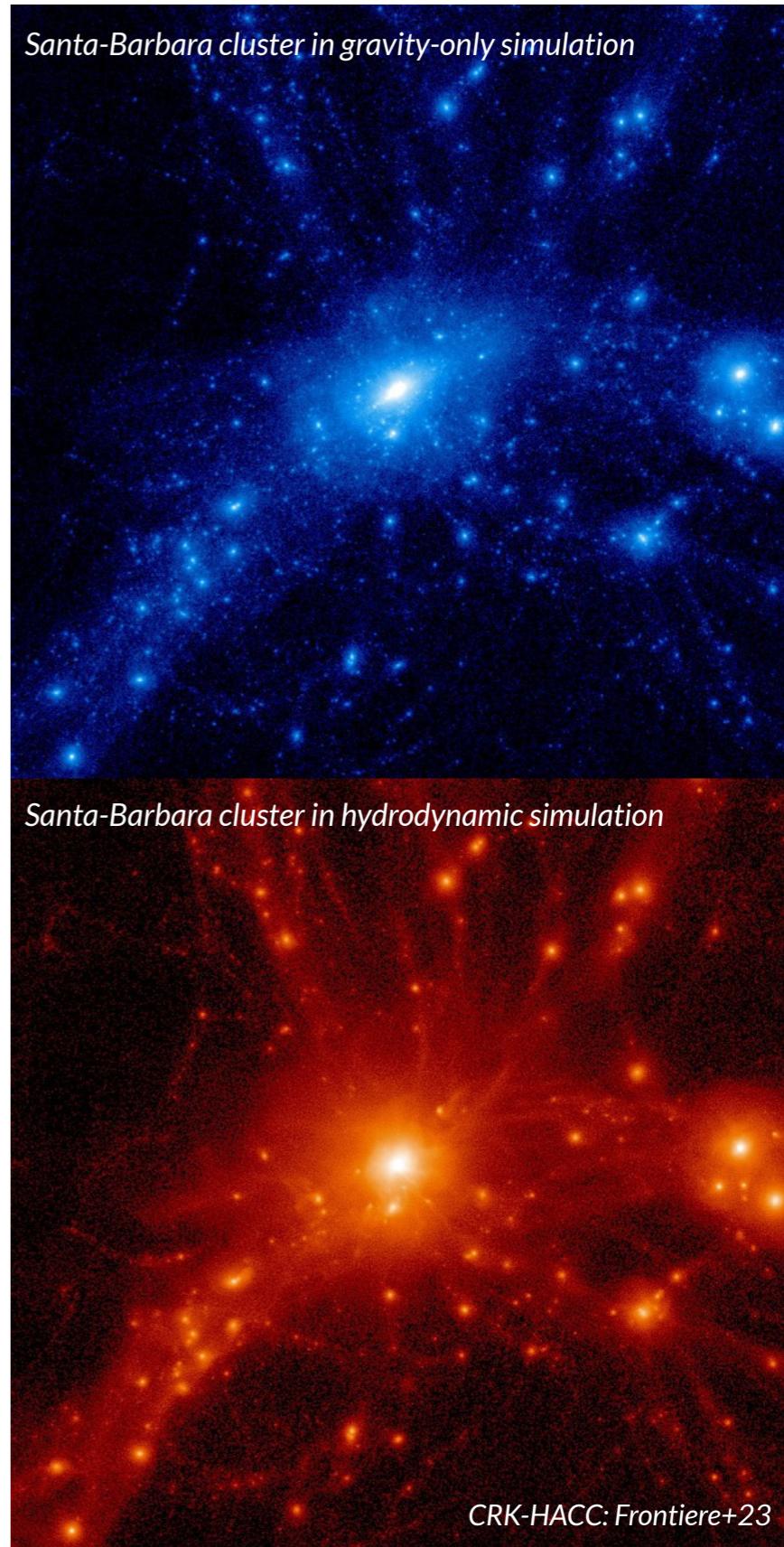
# Optimization and quality assessment of baryon pasting for intracluster gas

Florian Kéruzoré, Argonne National Laboratory  
mmUniverse23, June 2023

Kéruzoré et al., Submitted to OJA, arXiv:[2306.13807](https://arxiv.org/abs/2306.13807) (as of yesterday!)

# Context: Cosmological simulations for cluster science

- **Cluster cosmology needs simulations**  
*HMF calibration, accuracy/precision of mass estimates, selection functions, ...*
- Two types of cosmological simulations:
  - **Hydrodynamic:** Universe with CDM + baryons
  - **Gravity-only (GO):** All matter is CDM
    - ☺ ~10x faster than hydro  
→ larger volumes, more cosmologies
    - ☹ No baryons = no SZ (or X-rays)  
→ Can't produce all cluster observables
- **Baryon pasting (BP):** add gas a posteriori to create observables from GO simulations  
→ Get the products of a hydro simulation, for the price of a GO simulation
- **This work:** optimize baryon pasting to reproduce results from hydro simulations



# ANL cosmological simulations

- ANL produces state-of-the-art simulations using the HACC solver (*Habib+16, Frontiere+23*)

- **Large variety of available data:**

- Cutting-edge large boxes  
*OuterRim, LastJourney, FarPoint*
- Cosmo params hypercube  
*Mira-Titan*
- Volumes simulated in hydro and GO  
*BorgCube*

- Post-processing pipeline can produce:

- kSZ / simple tSZ from baryon pasting (*Flender+16*)
- Galaxies (*LSSTDESC+21*)
- (CMB) lensing maps (*Larsen+ in prep.*)

- **Widely used for cosmology** (e.g. LSST DC2)

- To be improved with DOE's exascale computers  
(*Aurora, Frontier*)

Year	Simulation	Code, Algorithm	Supercomputer, Location	Cores [10 <sup>3</sup> ]	$N_p$ [10 <sup>12</sup> ]	Box [ $h^{-1}$ Gpc]
2014	Dark Sky (Skillman et al. 2014)	2HOT FMM	Titan USA	20	1.1	8
2017	TianNu (Emberson et al. 2017)	CUBEP <sup>3</sup> M PM-PM-PP	Tianhe-2 China	331	2.97	1.2
2017	Euclid Flagship (Potter et al. 2017)	PKDGRAV3 Tree-FMM	PizDaint Switzerland	4	2.0	3.
2019	Outer Rim (Heitmann et al. 2019)	HACC Tree-PM	Mira USA	524	1.07	3.0
2019	Cosmo- $\pi$ (Cheng et al. 2020)	CUBE PM-PM	$\pi$ 2.0 China	20	4.39	3.2
2020	Uchuu (Ishiyama et al. 2021)	GREEN Tree-PM	ATERUI-II Japan	<40	2.0	2.0
2020	Last Journey (Heitmann et al. 2021)	HACC Tree-PM	Mira USA	524	1.24	3.4
2021	Far Point (Frontiere et al. 2021)	HACC Tree-PM	Summit USA	?	1.86	1

Table 1 List of cosmological simulations with a particle number in excess of 1 trillion (10<sup>12</sup>)

Angulo+23



- **Context**
- **Optimizing baryon pasting vs hydrodynamic simulations**
  - The Borg Cube simulations
  - Model & Optimization method
  - Results
- **Quality assessment**
  - Gas profiles
  - Preliminary fixed-z tSZ products
- **Conclusions, outlook**

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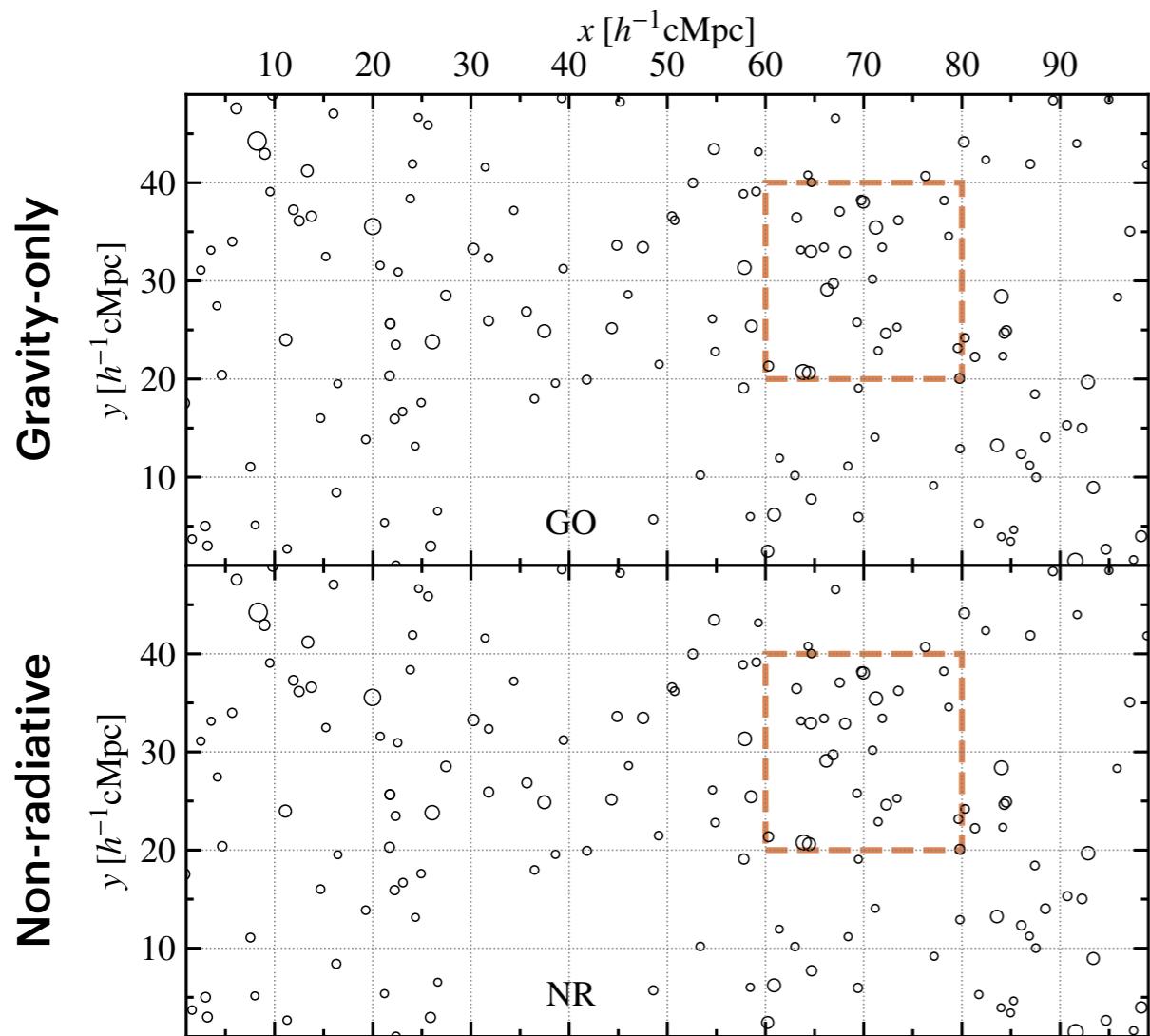
# The Borg Cube simulation(s)

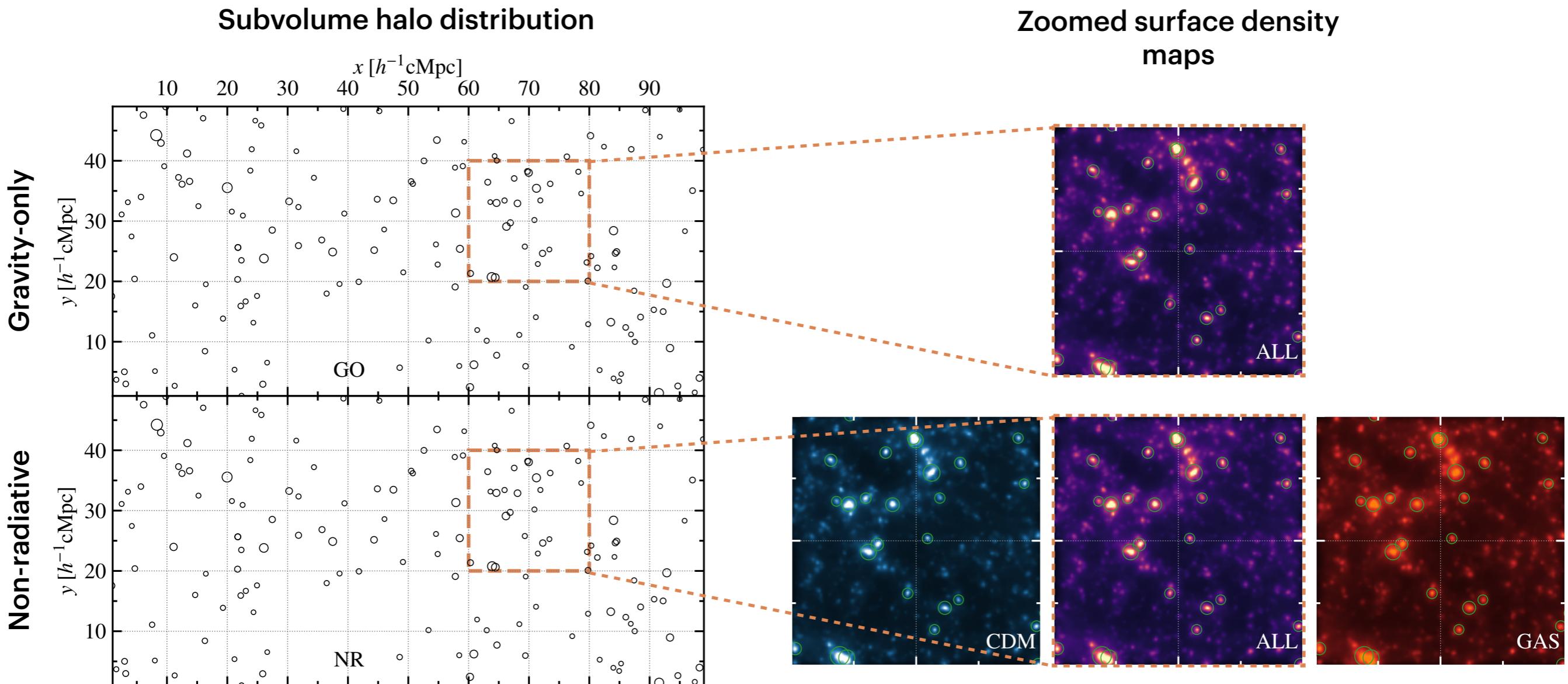
- Volume =  $(800 h^{-1} \text{cMpc})^3$ ; particle mass  $\sim 10^9 h^{-1} M_\odot$
- Two simulations with same initial conditions:
  - **GO:** Gravity-only
  - **NR:** Non-radiative hydro  
*First CRK-HACC hydrodynamic simulation (Emberson+19)*

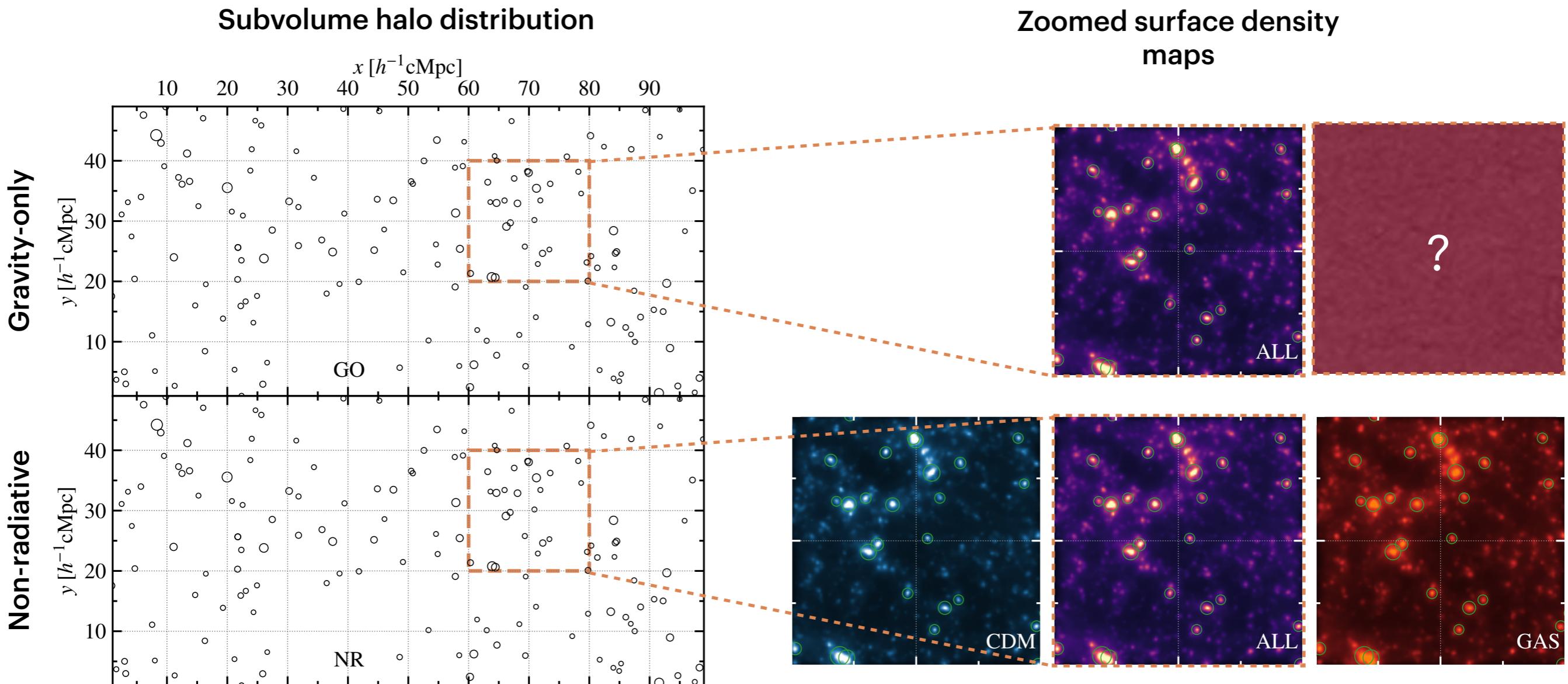
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  - Two simulations with same initial conditions:
    - **GO:** Gravity-only
    - **NR:** Non-radiative hydro
-  Same initial conditions → ~ same halos
- First CRK-HACC hydrodynamic simulation (Emberson+19)*

## Subvolume halo distribution



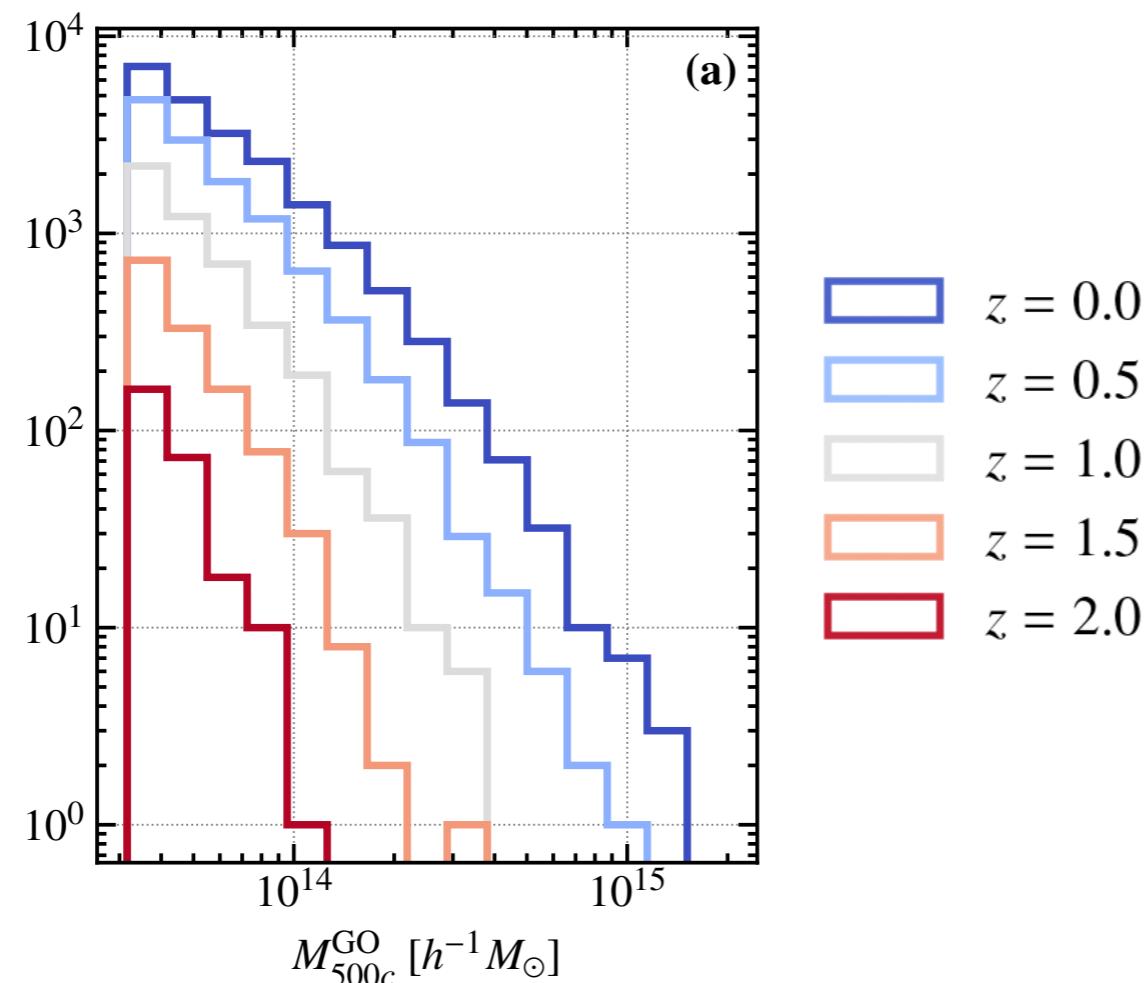




→ How can we reproduce the NR gas distribution from the GO matter distribution?

# Halo sample: cluster-scale, matched in both runs

- Study cluster-scale halos:  $M_{500c} \geq 10^{13.5} h^{-1} M_\odot$
- Match halos in both runs based on distance + similar mass
  - >98% of GO halos are matched



Redshift	$N_{\text{halos}}^{\text{GO}}$	$N_{\text{halos}}^{\text{both}}$
$z = 0$	20458	20120
$z = 0.5$	11880	11703
$z = 1$	4698	4644
$z = 1.5$	1315	1311
$z = 2$	263	260
Total	38614	38038

- **Model:** based on Ostriker+05 model: for 1 halo, BP gas density & pressure fixed by:
  - GO 3D grav. potential
  - Model parameters:
    - gas polytropic index  $\Gamma$ ,
    - fraction of CDM energy transferred to gas  $\varepsilon_{\text{DM}}$(see D. Nagai's talk)
- **Optimization workflow:**
  - Run baryon pasting on all halos, on a grid of parameter values:  
 $\Gamma \in [1.13, 1.20]$ ;  $\varepsilon_{\text{DM}} \in [0, 5\%]$
  - For each halo, compare relative difference between BP and NR gas density and pressure,

$$\chi_\rho = \frac{\rho_g^{\text{BP}}}{\rho_g^{\text{NR}}} - 1, \quad \chi_P = \frac{P_g^{\text{BP}}}{P_g^{\text{NR}}} - 1$$

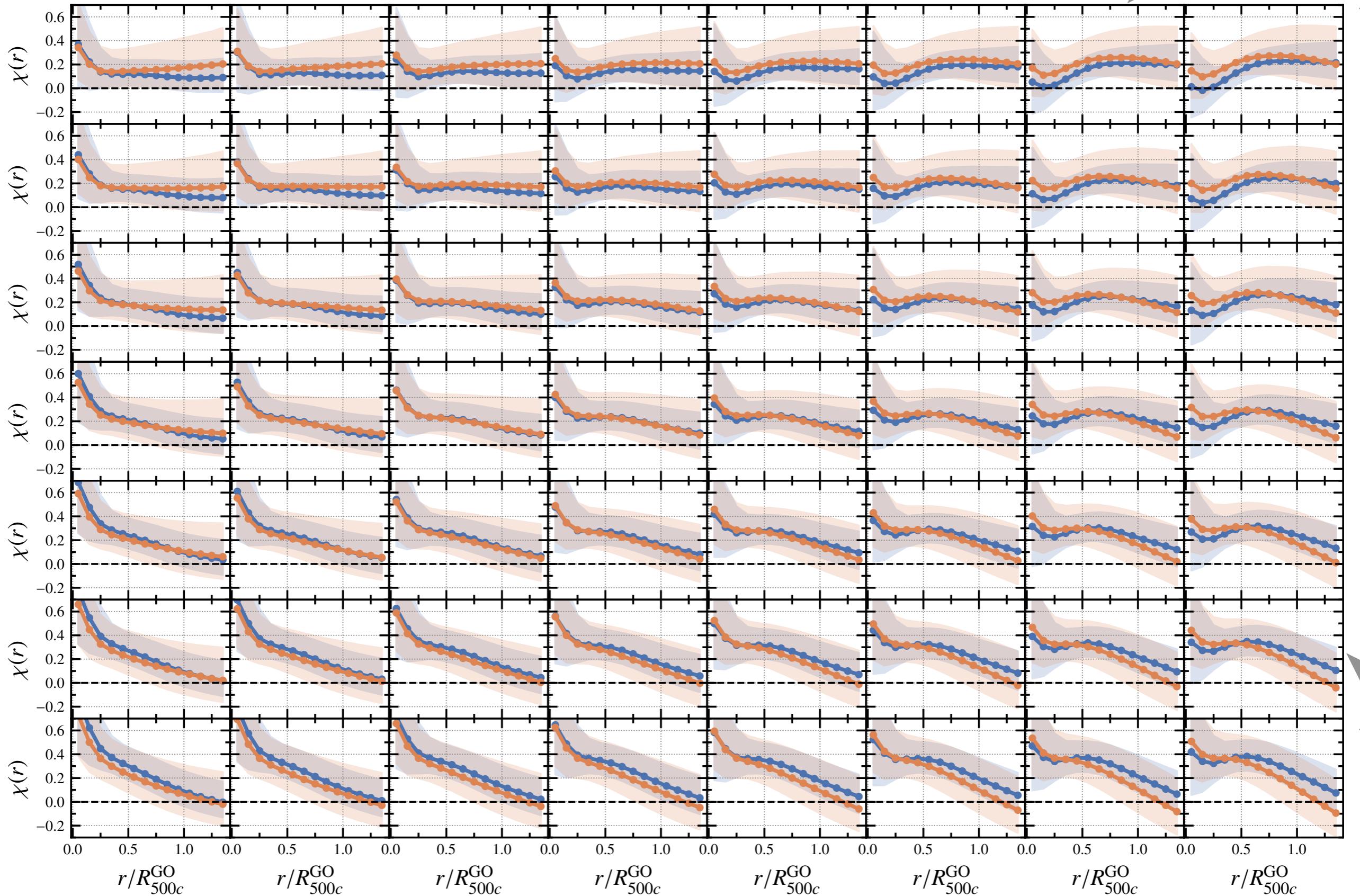
- Compute the radial profiles of  $(\chi_\rho, \chi_P)$  for all halos
- Repeat for all redshifts independently

# Results: z=0 (n=20,120)

Blue: Density   Orange: Pressure

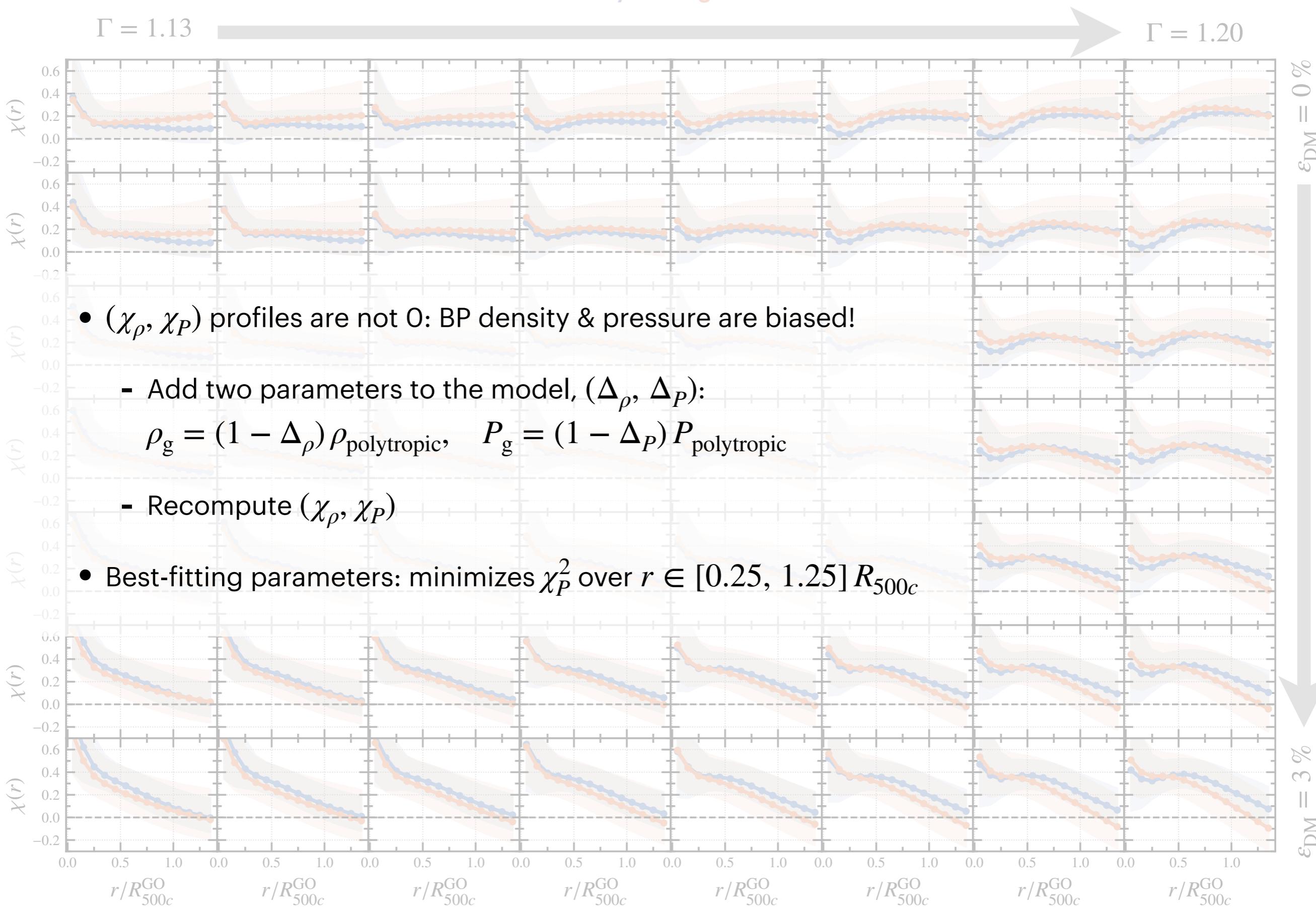
$\Gamma = 1.13$

$\Gamma = 1.20$

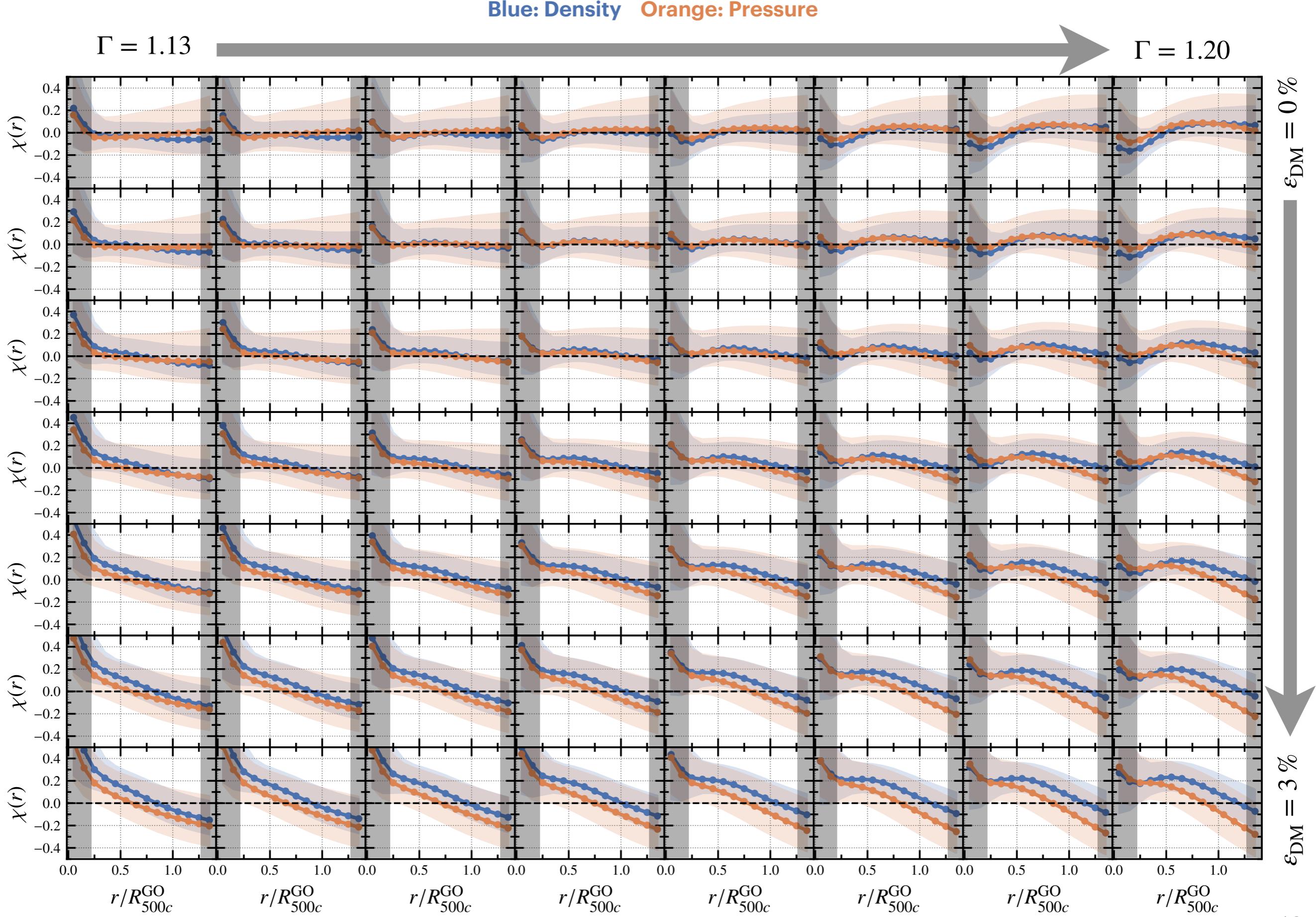


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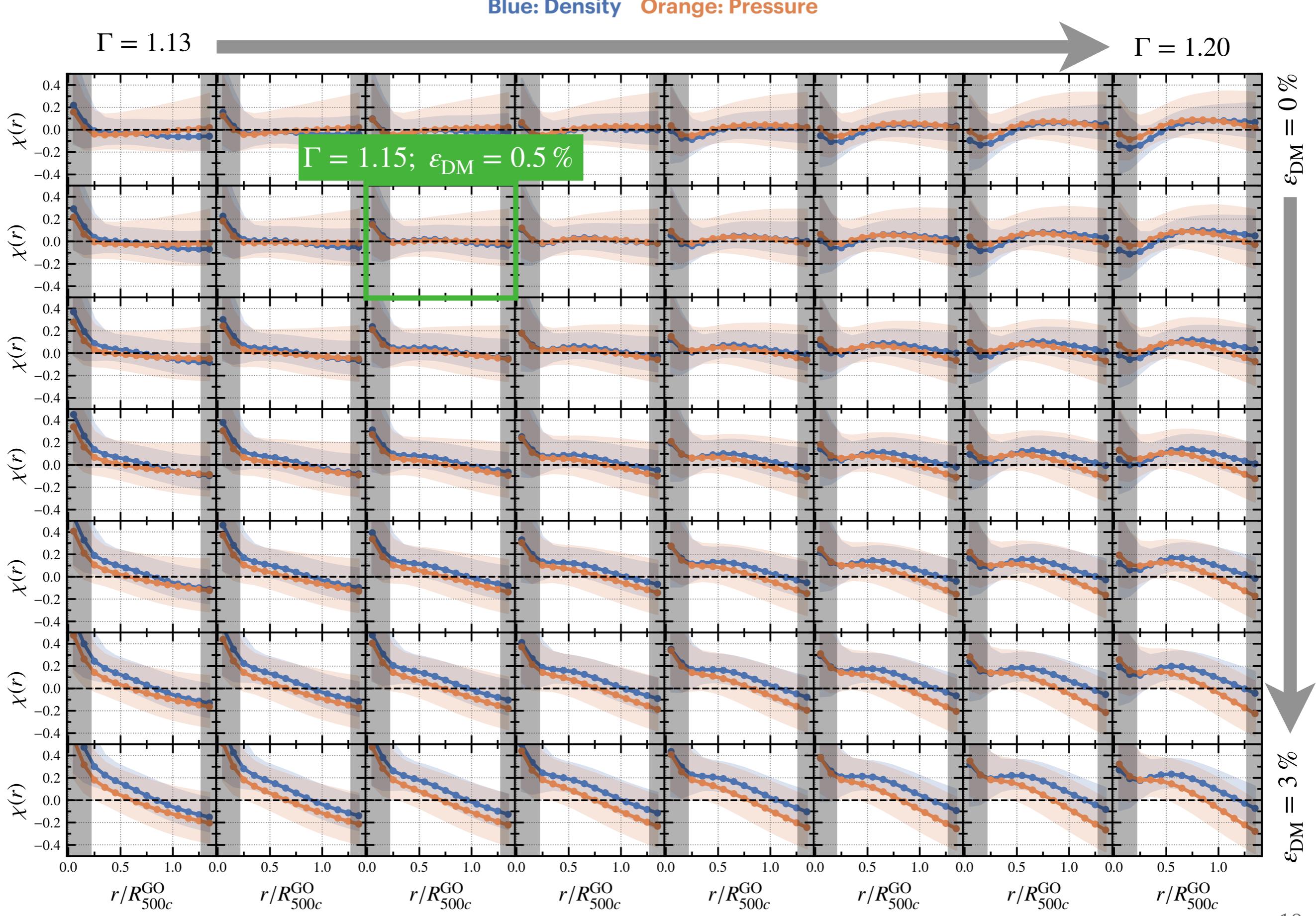
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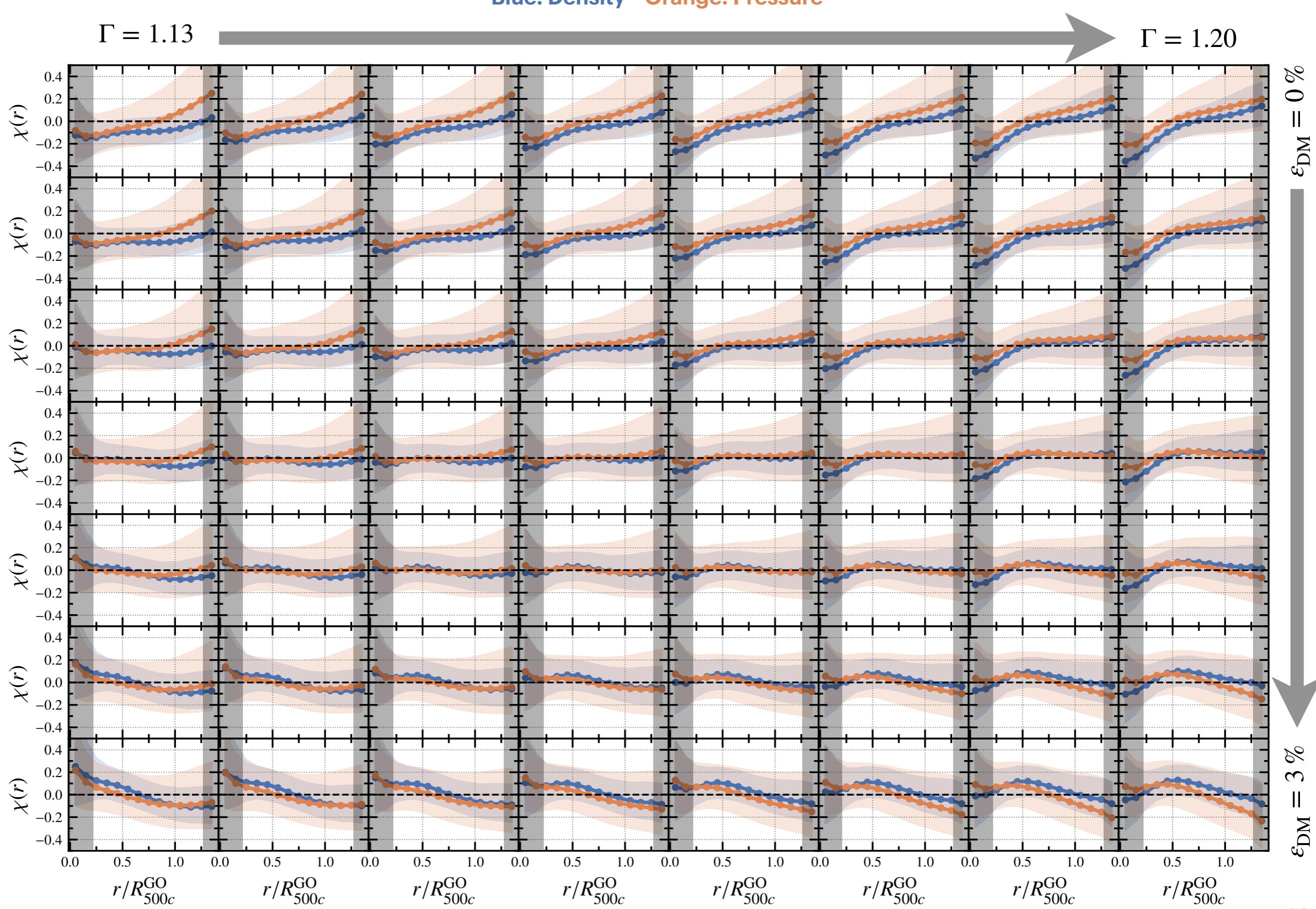
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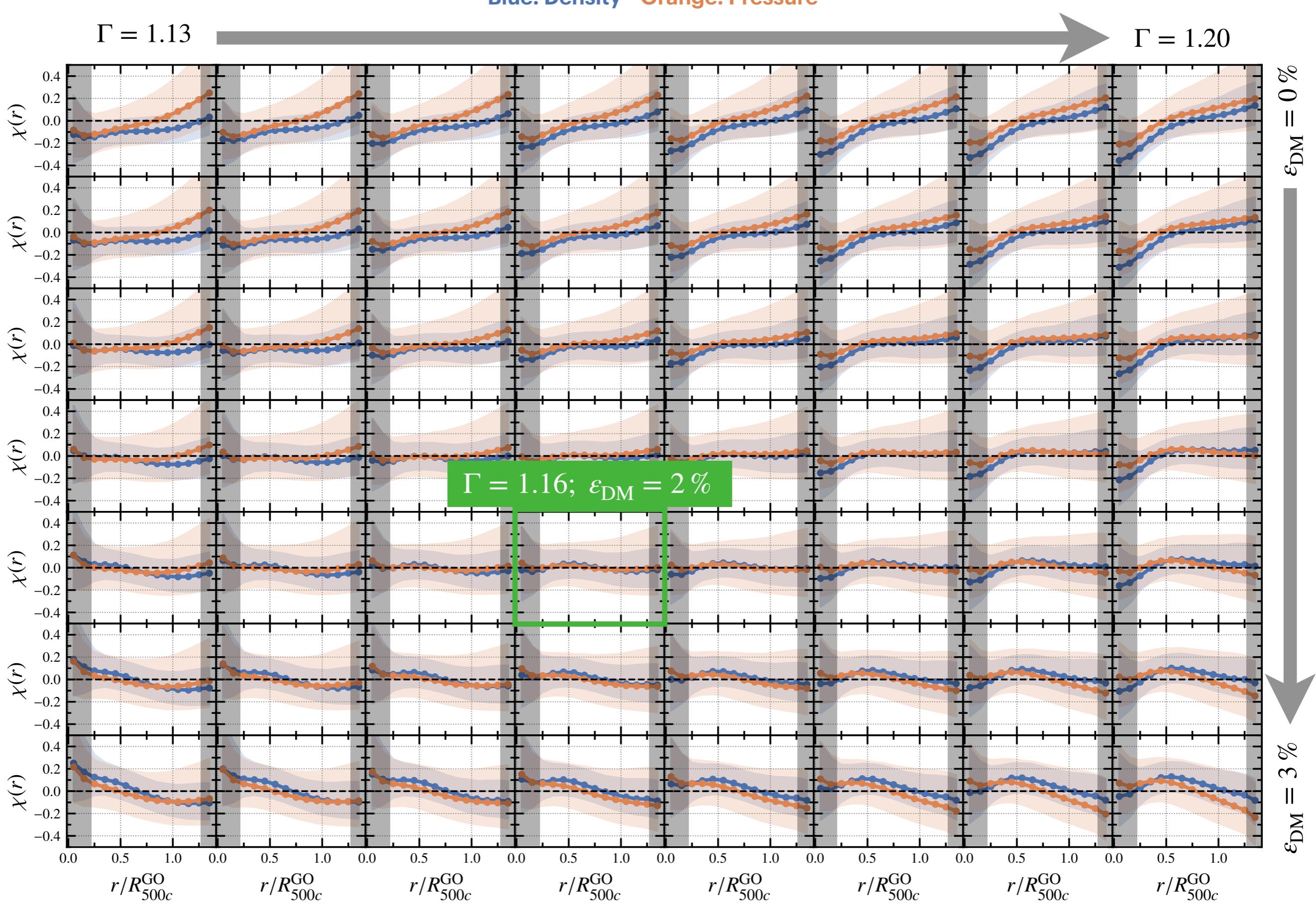
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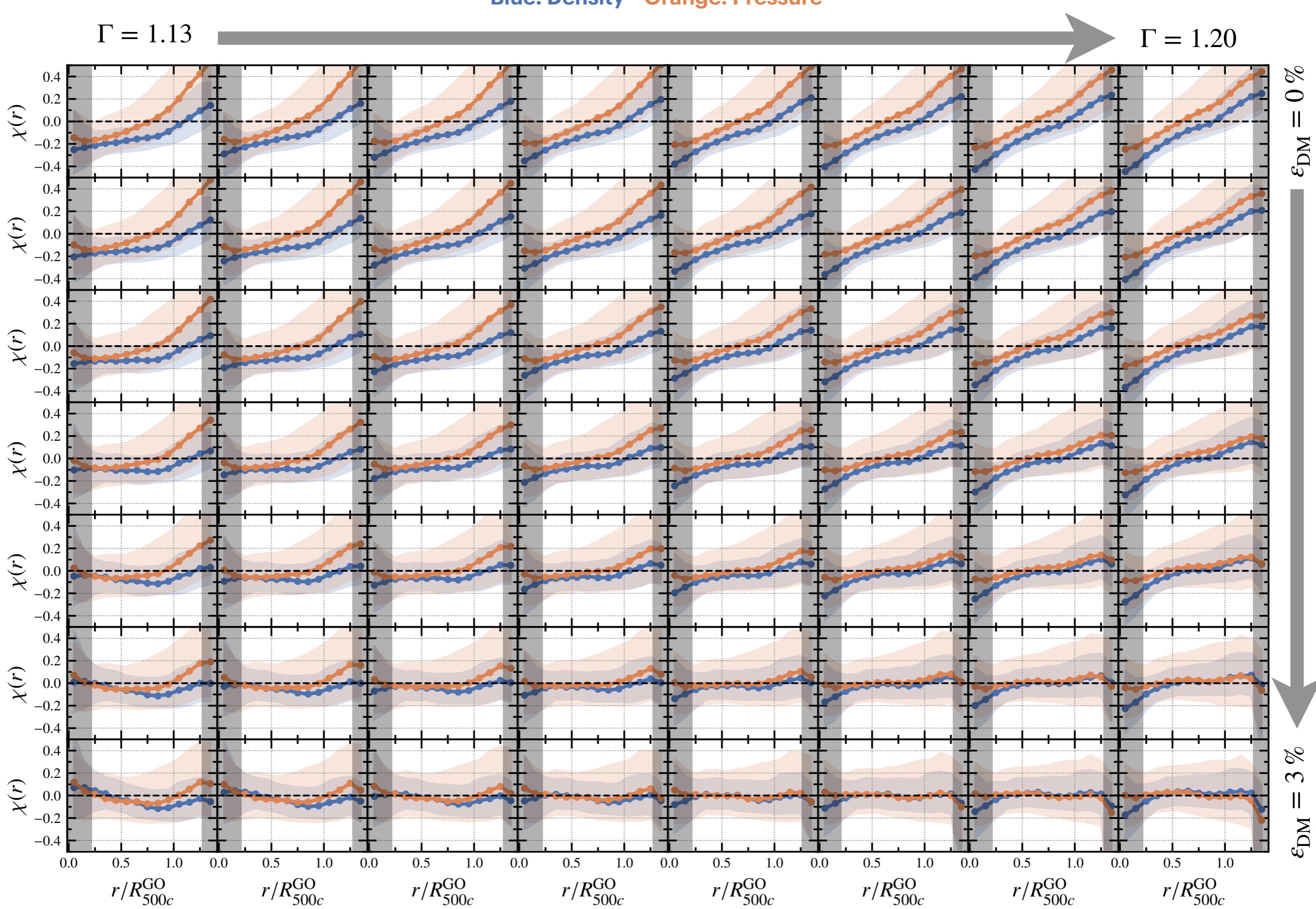
# Results: z=1 (n=4,644)



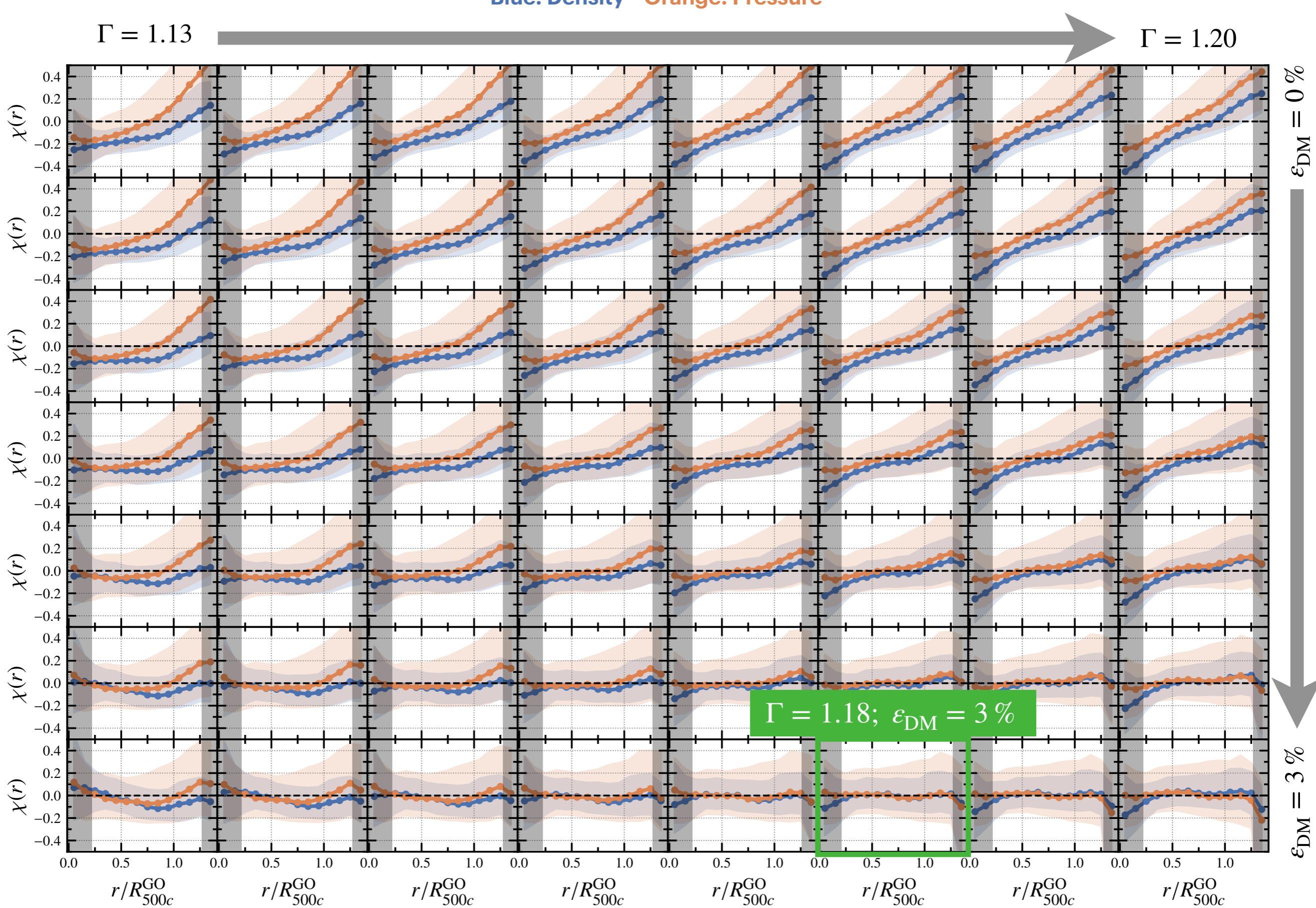
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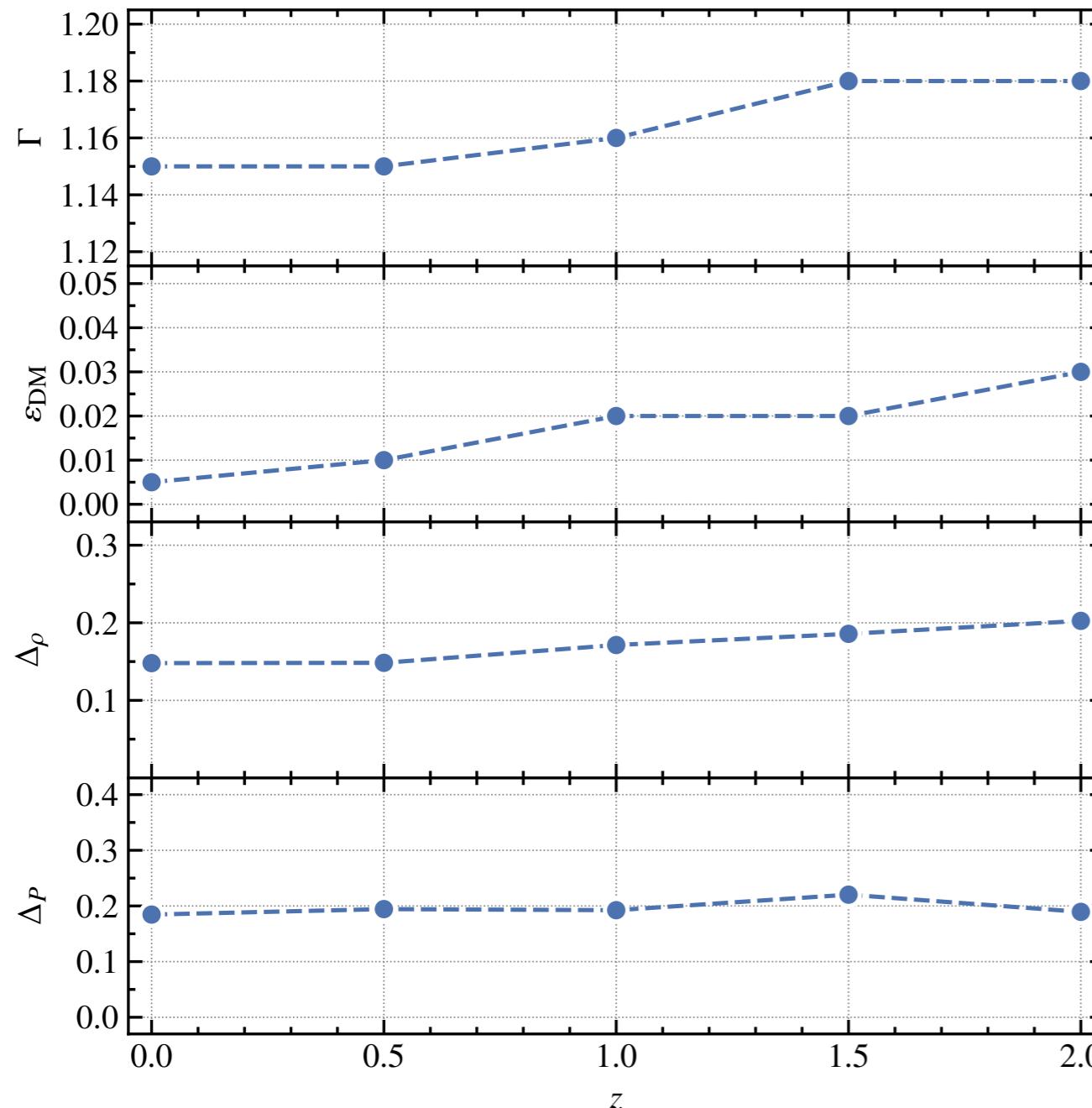
# Results: $z=2$ ( $n=260$ )



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# Results: params = f(z)

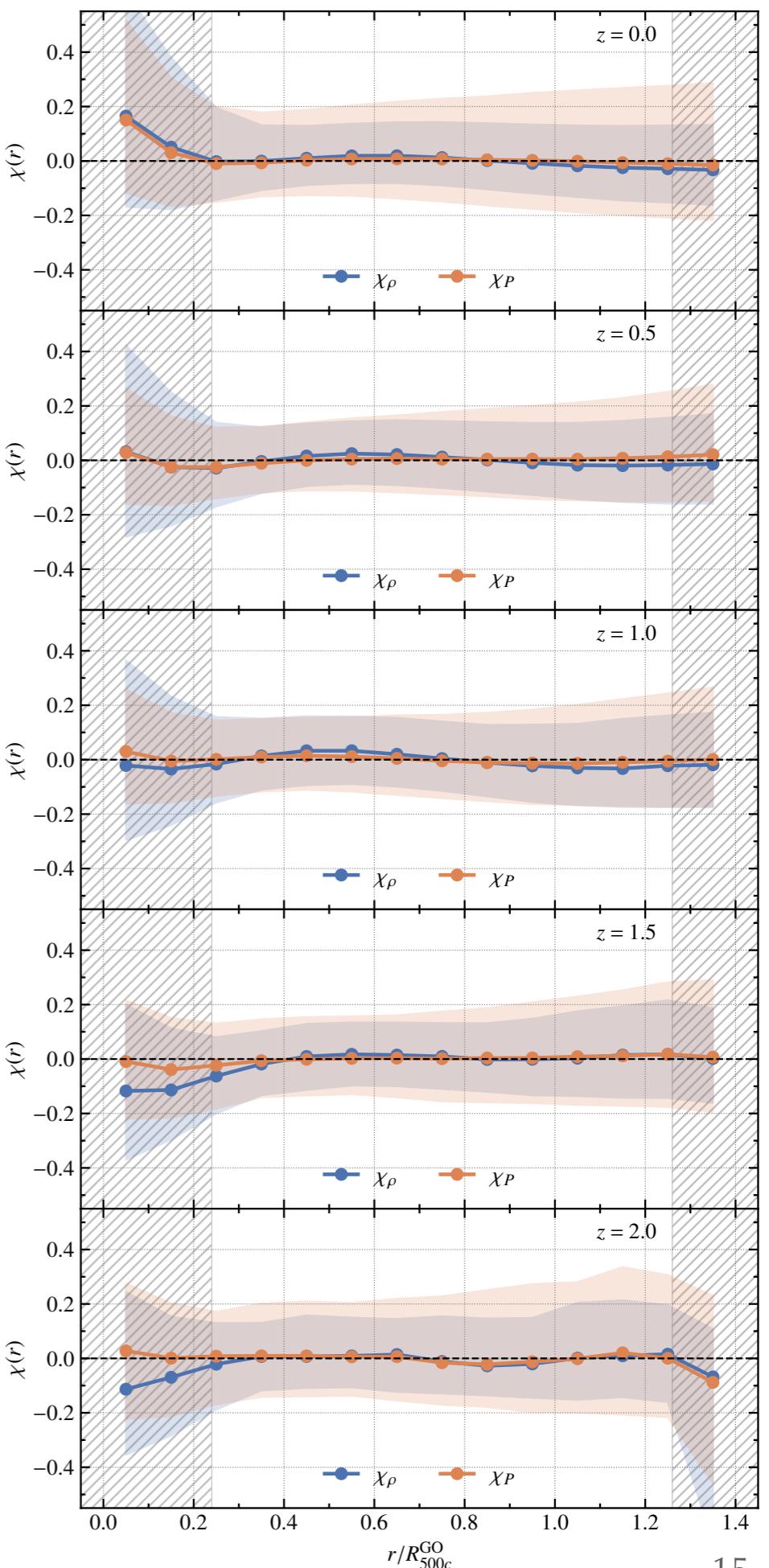


- Measured redshift trend in  $(\Gamma, \varepsilon_{\text{DM}})$ 
  - $\Gamma(z = 0) = 1.15$   
 $\rightarrow \Gamma(z = 2) = 1.18$
  - $\varepsilon_{\text{DM}}(z = 0) = 0.5 \%$   
 $\rightarrow \varepsilon_{\text{DM}}(z = 2) = 3 \%$
- Measured bias parameters:
  - Density:  $\Delta_\rho \sim 15 - 20 \%$
  - Pressure:  $\Delta_P \sim 20 \%$

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# Gas profiles reconstruction: accuracy & precision

- Agreement between density and pressure
- For the best parameters at each  $z$
- Focusing on  $r \in [0.25, 1.25] R_{500c}$
- Accuracy:
  - $< 3\%$  on pressure
  - $< 2\%$  on density
- Scatter:
  - Radially dependent
  - $\sim 20\%$  on pressure
  - $\sim 15\%$  on density

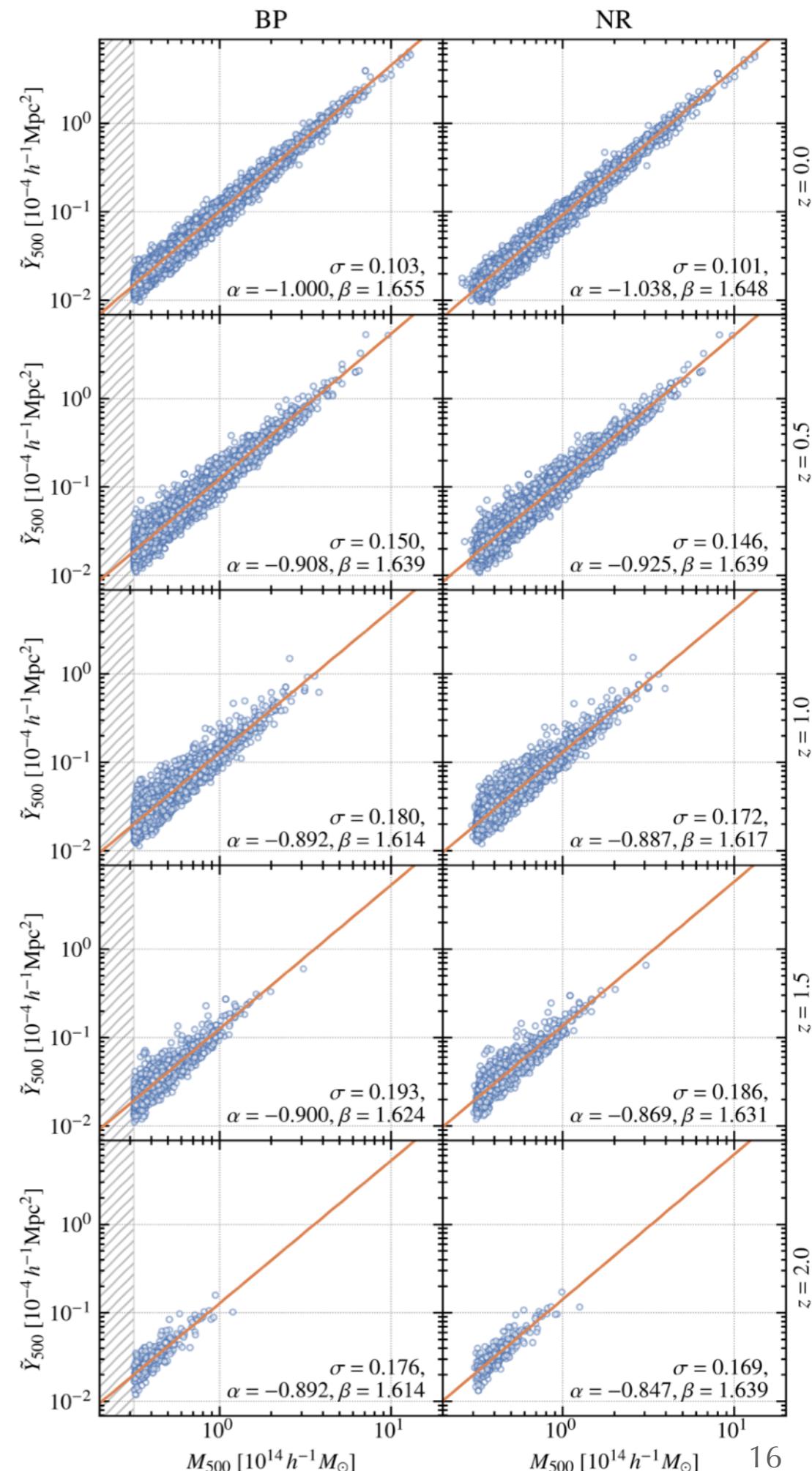


# $Y_{500} | M_{500}$ scaling relation reconstruction

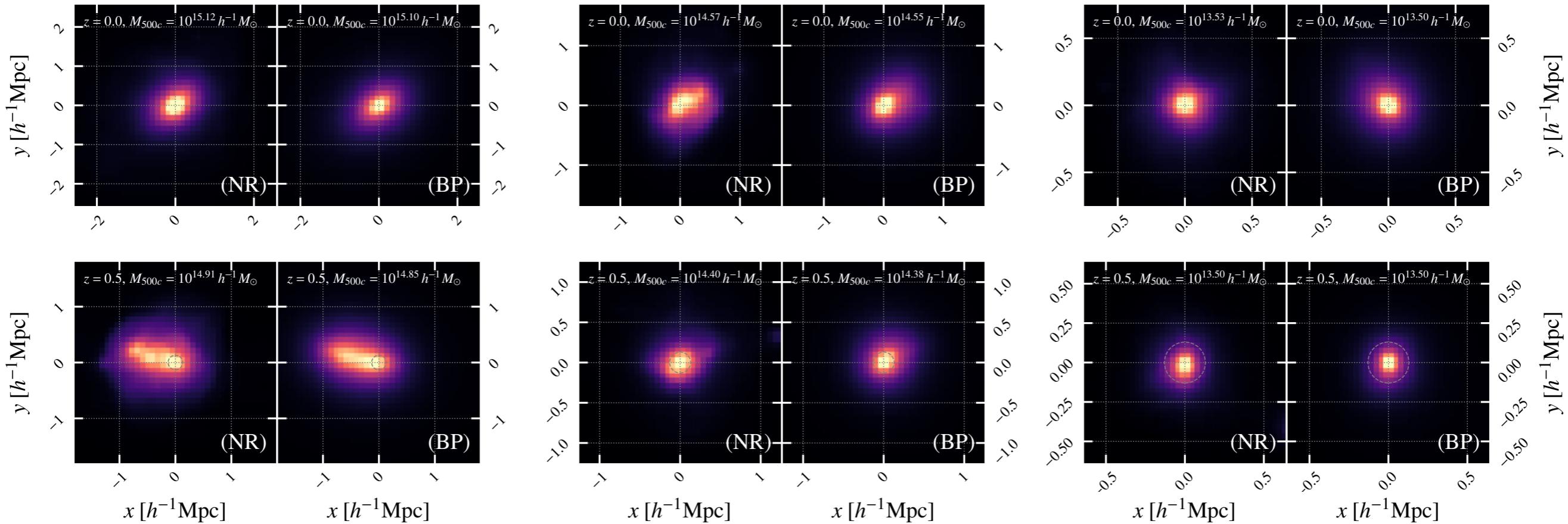
- $Y|M$ : important tool for cluster cosmology  
(See talks by L. Bleem, L. Salvati, L. Perotto, G. Aymerich, A. Moyer, A. Paliwal, ...)

$$E^{-2/3}(z) \frac{D_A^2 Y_{500}}{10^{-4} h^{-1} \text{Mpc}^2} = 10^\alpha \left[ \frac{M_{500}}{3 \times 10^{14} h^{-1} M_\odot} \right]^\beta + \mathcal{N}(0, \sigma^2)$$

- Compare  $Y|M$  from BP (left) vs NR (right):
  - Similar reconstructed parameters
  - Extra scatter due to baryon pasting:  
 $< 5\%$  of NR scatter

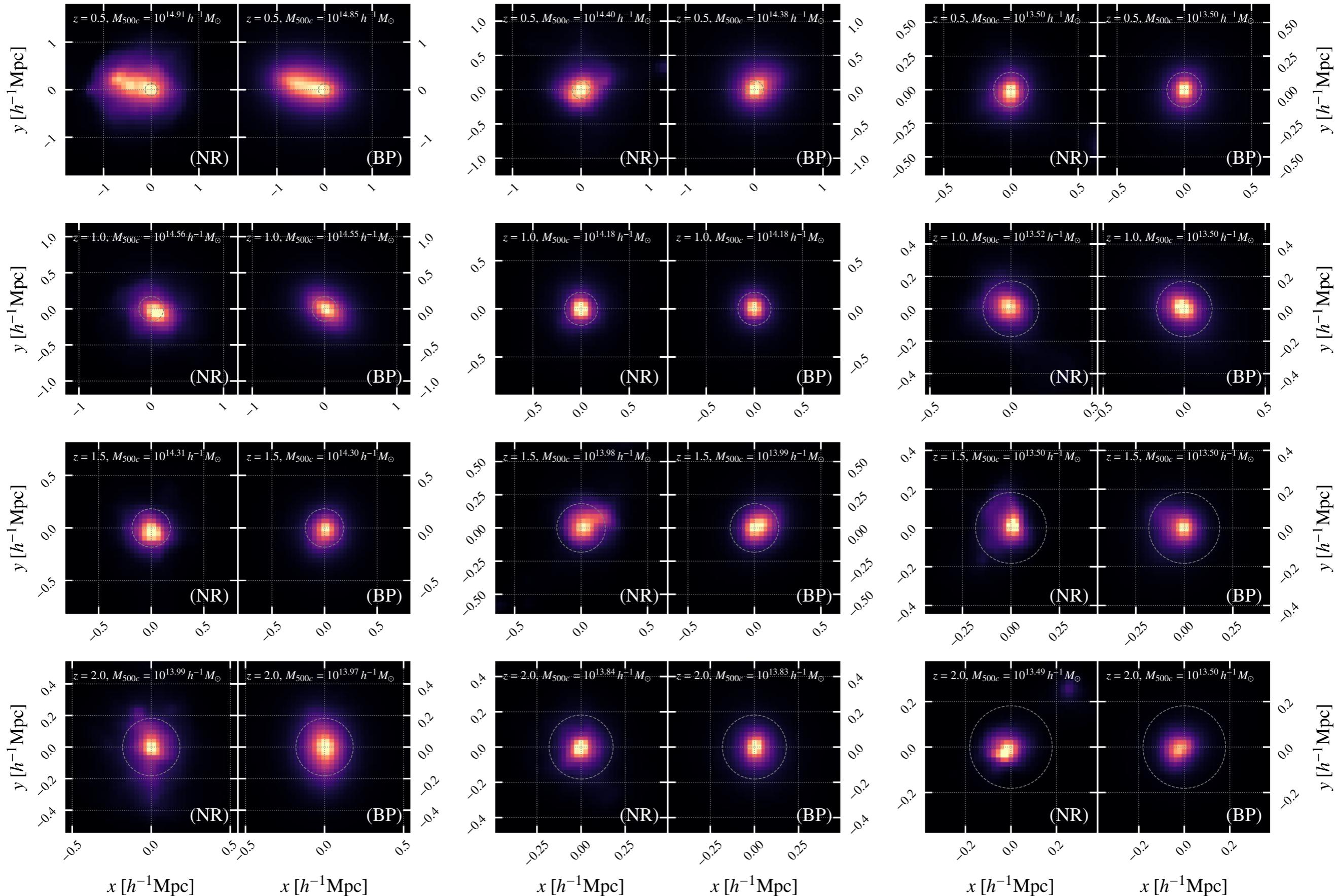


# First look at tSZ thumbnails: $z=0$ , $z=0.5$



- Side-by-side tSZ map of matched halos, in NR (left) & BP (right)
  - Global shape & tSZ amplitude well reconstructed
- $z > 0$ : circle = 1 arcmin (typical resolution of ground-based CMB surveys)

# First look at tSZ thumbnails: $z > 0$



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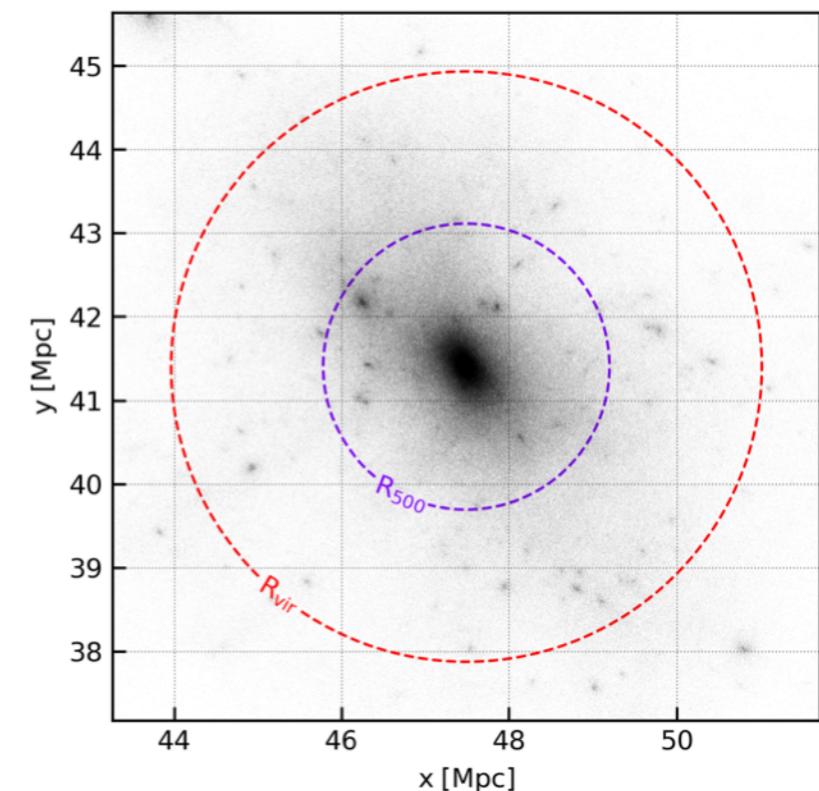
- Progress towards baryon pasting pipeline for HACC GO simulations
- Optimized Ostriker+05 model to reproduce hydrodynamic simulation:
  - From direct per-halo comparison on ~40,000 halos, for  $z \in [0, 2]$
  - Redshift trend observed in model parameters
- Results: using a gravity-only simulation, up to  $z = 2$ ,
  - Pressure / density reconstructed with ~few % accuracy, ~20% scatter
  - $Y_{500} | M_{500}$  scaling relation well reconstructed, with <5% excess scatter
  - First look at maps: tSZ amplitude / shape reconstructed

- **Systematic application to HACC gravity-only simulations**
  - OuterRim (DESC cosmoDC2 Universe)
  - Mira-Titan (111 simulations with varying cosmology)
  - +all cosmological volumes (Last Journey, Farpoint, ...)
- **Model extension:**
  - This work omits subgrid physics (cooling, star formation, feedback)
  - Absent from the Borg Cube; recently implemented in HACC  
*CRK-HACC, Frontiere+23*
  - Same analysis to be repeated on newer complete hydro sims
  - Observational data to be used for further validation

# Backup

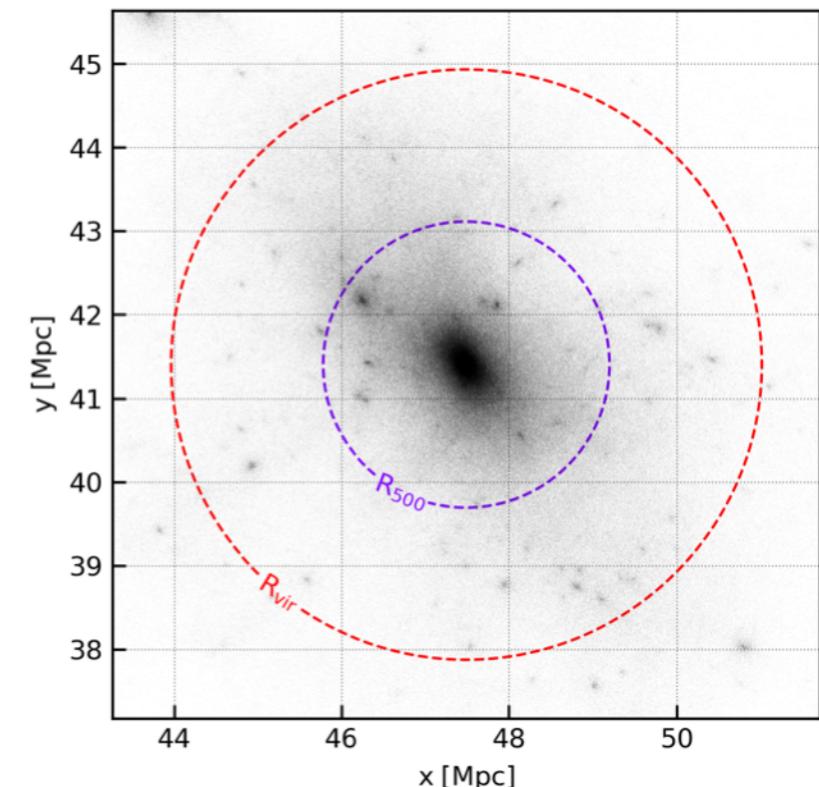
# Baryon pasting model

- Model based on Ostriker+05 (see D. Nagai's talk)
- Input data: for one halo,  $(M_{\text{vir}}, R_{\text{vir}})$  + particles
  - Assume polytropic equation of state:
  - $\rho_g = \rho_{g,0} \theta(\phi)^{\Gamma/(\Gamma-1)}$ ;  $P_g = P_{g,0} \theta(\phi)^{1/(\Gamma-1)}$
  - $\theta(\phi)$ : fixed from GO grav. potential
  - $\Gamma$  : gas polytropic index (fixed model parameter)
  - $(\rho_{g,0}, P_{g,0})$  : central gas density/pressure, TBD



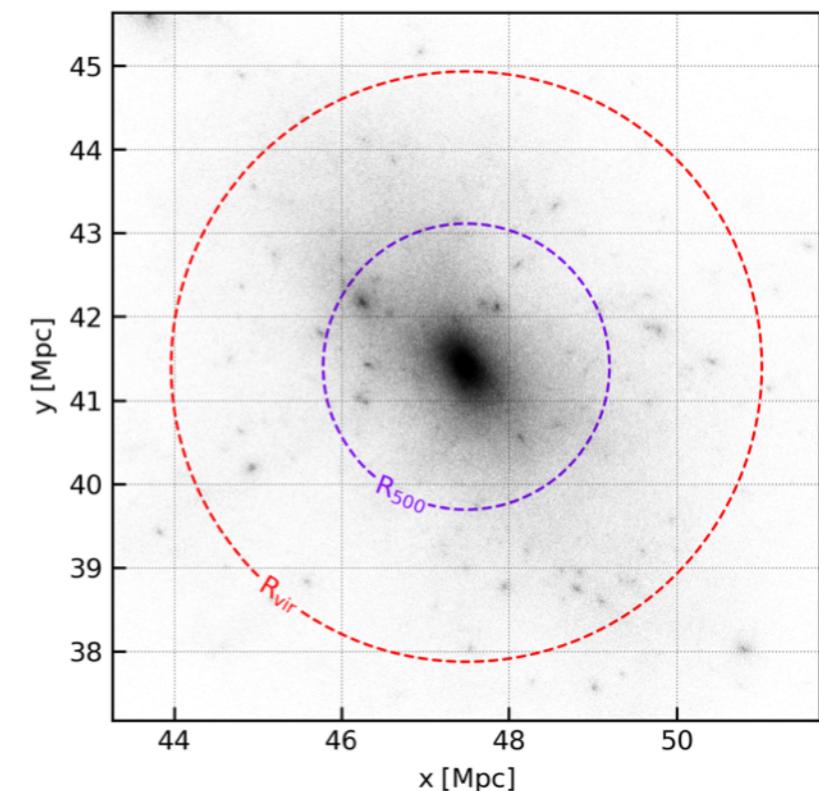
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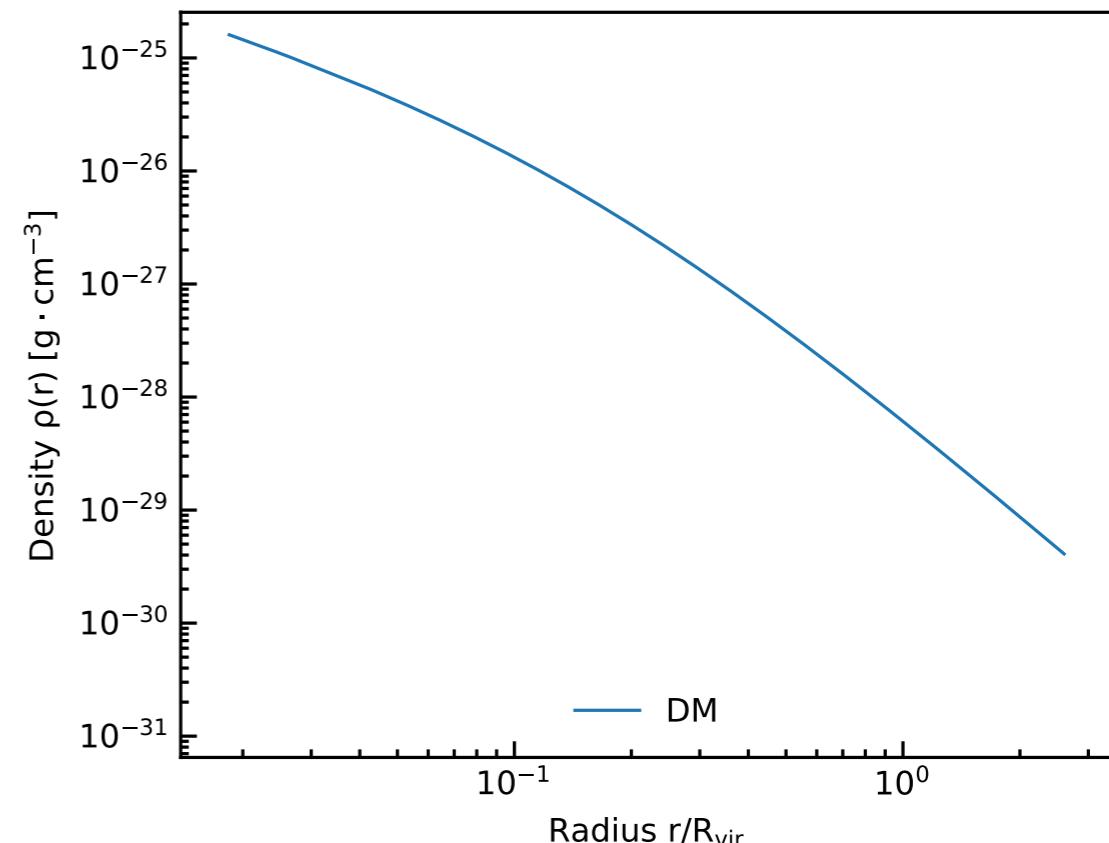
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  - Assume gas rearrangement



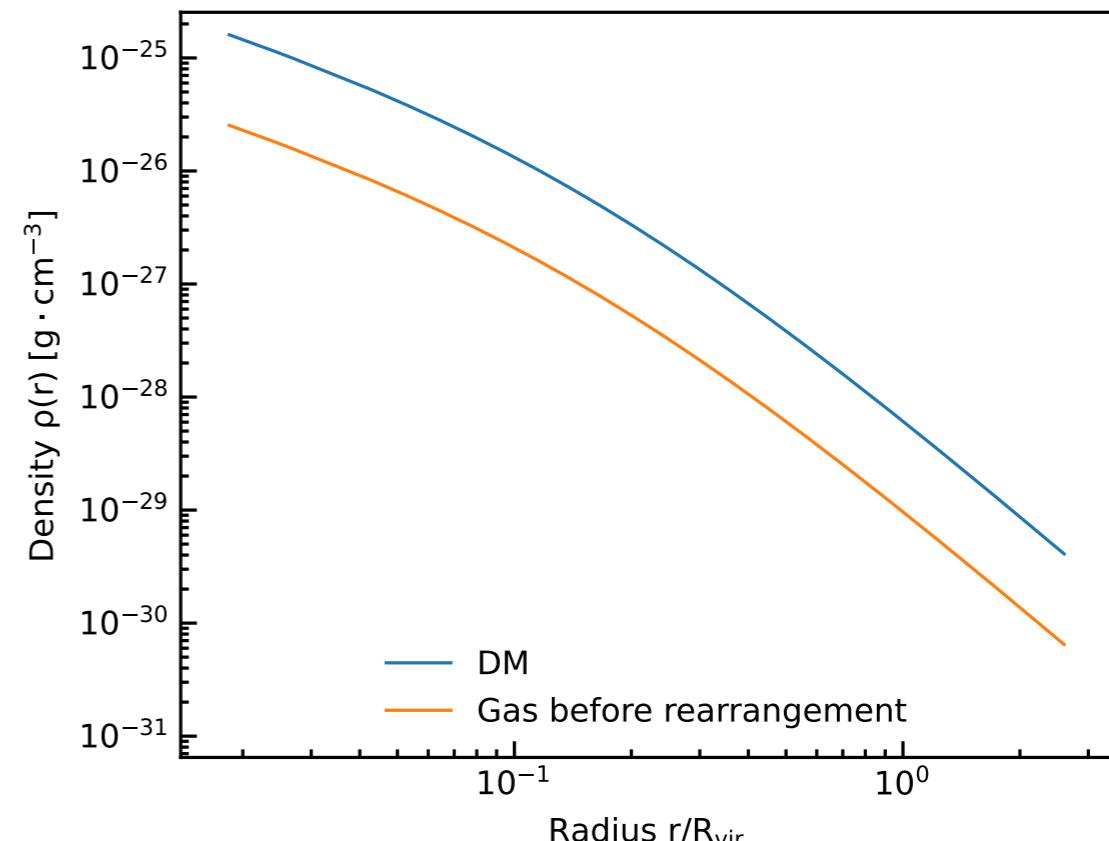
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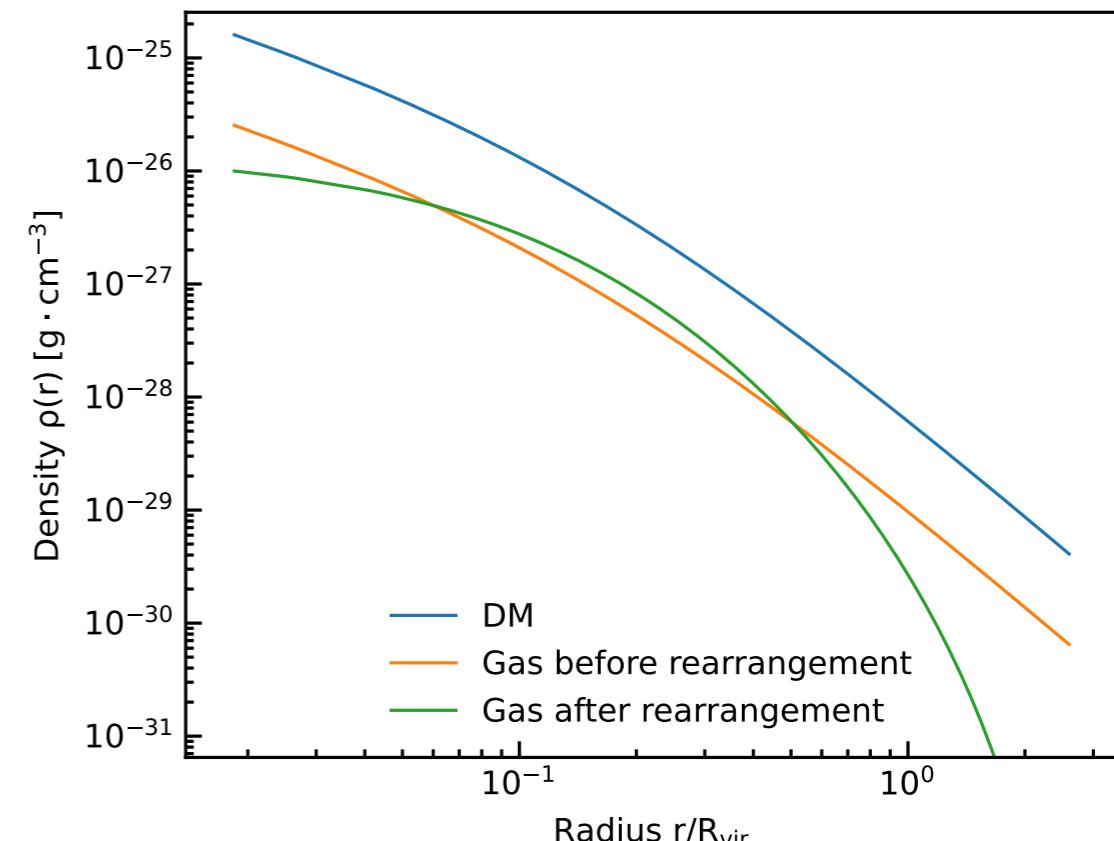
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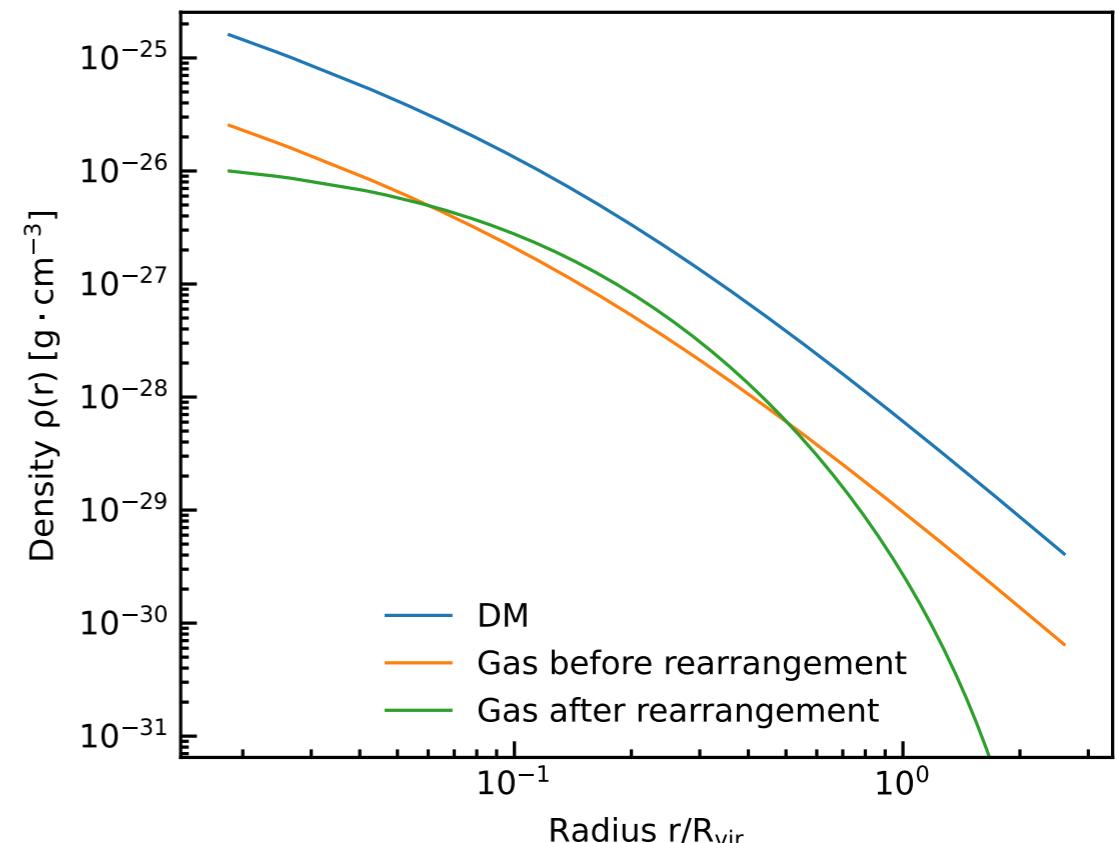
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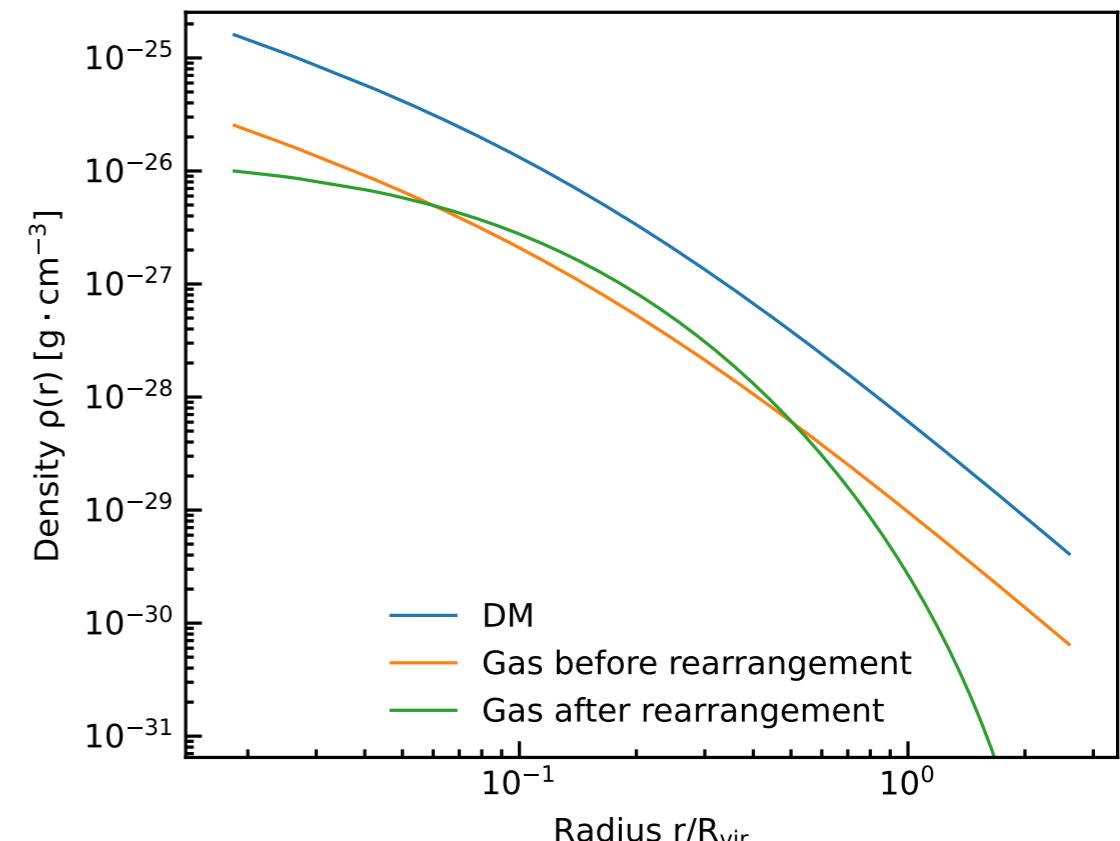
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  - Conserving surface pressure / gas energy
  - A fraction  $\varepsilon_{\text{DM}}$  of CDM energy is transferred to gas (fixed model parameter)



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→ For one halo, gas props fixed by GO particles + 2 model parameters:  $(\Gamma, \varepsilon_{\text{DM}})$

# Scatter in gas properties = scatter in mass?

- Part of the scatter on  $(\rho, P)$  is scatter on  $M_{500c}$  :
  - Cluster more (less) massive in hydro  
→ Has more (less) gas in hydro
  - $M_{500c}^{\text{NR}} | M_{500c}^{\text{GO}}$  has scatter → induced scatter in  $(\rho, P)$

