Advancements in the modeling of cluster statistics

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IFPU - Focus Week
The astrophysics of large-scale structures in the era of eROSITA, Euclid, SPT-3G: the emergence of the cosmic web

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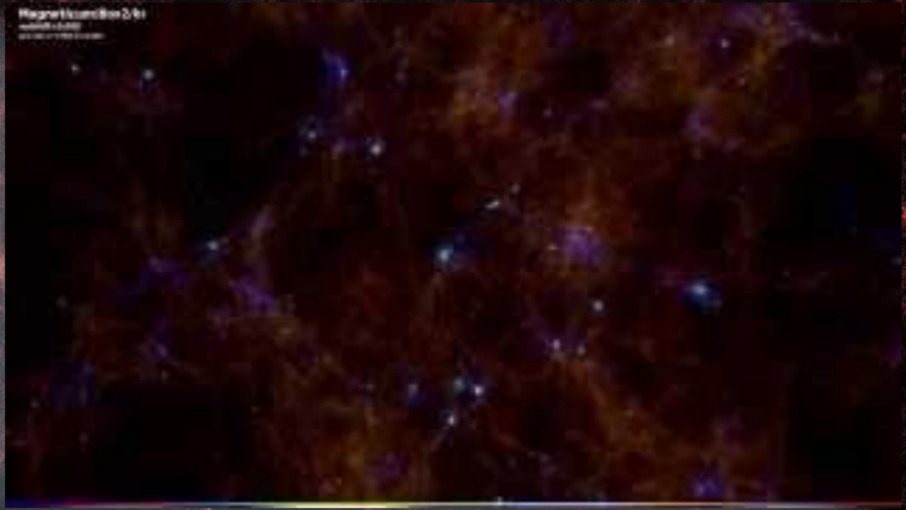
Outline

- Numerical cosmology
  - Introduction to Cosmological Simulations
  - HMF calibration in LCDM (Euclid Collaboration: Castro et al. 2023)
  - *N*-Body simulations with DDE
  - *N*-Body simulations with CDE
- Modelling the HMF
  - Dynamical Dark Energy (Euclid Collaboration: Castro et al. 2023, Castro et al. 2025a)
  - Clustering Dark Energy (Castro et al. 2025a, Castro et al. 2025b)
- Modelling the Halo bias (Euclid Collaboration: Castro et al. 2024b)
- Effect of Baryons:
  - Dissecting the impact of baryons on halo masses (Castro et al. 2020)
  - Modeling the impact of baryons on halo masses (Euclid Collaboration: Castro et al. 2024a)
- Conclusions

Numerical Cosmology

Introduction to Cosmological Simulations

- Cosmological simulations are crucial in understanding the formation and evolution of the Universe.
- In the large-scale structure (LSS), gravity is the primary influence but does not act alone.
- Baryonic feedback, such as AGN and SNe feedback and gas cooling, although sub-dominant, are known to affect the LSS in a noticeable way.
- Baryonic feedback impact is at the focal point, as neglecting them could lead to biased cosmological constraints.



Introduction to Cosmological Simulations

N-Body simulations

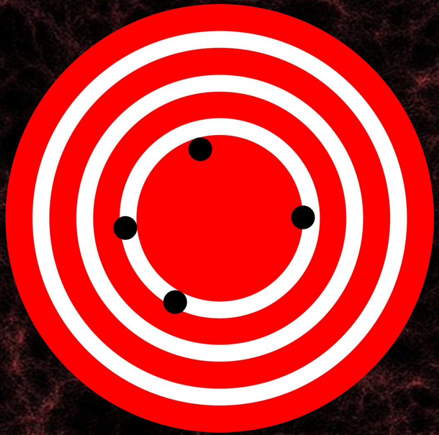
- Gravity is the only interactions.
- Universe represented by a finite number of particles.
- Calculate gravitational forces between particles.
- Track motion and evolution over time.
- Strengths and Limitations:
  - High precision and accuracy.
  - Lacks detailed baryonic matter interactions.

Hydro Simulations

- Simulate both dark matter and baryonic matter (gas, stars).
- Solve equations of hydrodynamics along with gravity coupling them to the SF and Feedback.
- Strengths and Limitations:
  - More comprehensive than *N*-body simulations.
  - Computationally more demanding (x 1000!).
  - **Sub-resolution modelling.**

The HMF: Numerical/Theoretical systematics

- Assessing the robustness of the simulations predictions is not an easy task:
  - For instance, tweaking code parameters and searching for convergence can result in inaccurate result.



Low accuracy and low precision

Low accuracy and high precision

The HMF: Numerical/Theoretical systematics

- Designing an accurate and precise set of simulations for Cluster Cosmology:

Set	$L_{\rm box}$ (h^{-1} Mpc)	$N_{\rm p}$	Background	$P_{\rm lin.}(k)$	Initial Conditions: Code	Initial Conditions: LPT Order	Initial Conditions: z	Grav. Solver
TEASE	500	256^3, 512^3, 1024^3, 4×160^3, 4×320^3, 4×640^3, 4×1280^3	$C0$	ΛCDM	MUSIC	Zel.	99	Tree-PM, FMM-PM, FMM, P^3M, AMR†
					monofonIC	3LPT	24	Tree-PM, FMM-PM, FMM, P^3M
AETIOLOGY	1000	1024^3	EdS	Power-law, ΛCDM ($C0$)	GADGET-4	2LPT	99	FMM-PM
			$C0$	Power-law, ΛCDM				
PICCOLO	2000	4×1280^3	$C0-C8$	ΛCDM	monofonIC	3LPT	24	Tree-PM

The HMF: Non-universality modelling

- We have adopted a bottom-up approach to develop our HMF model:
  - **Selecting the fitting-function to be calibrated using scale-free simulations;**
  - **Modelling the evolution of the parameters as a function of the matter power spectrum shape;**
  - **Using simulations with composed initial conditions to discriminate between the impact of the background evolution and the matter power spectrum shape.**

$$f(\nu) = f_{\mathrm{ST}}(\nu)(\nu\sqrt{a})^{q-1}$$

$$f_{\mathrm{ST}}(\nu) = A\sqrt{\frac{2a}{\pi}}\nu e^{-\frac{a\nu^2}{2}}\left(1+(a\nu^2)^{-p}\right)$$

$$q = q_R \times \Omega_m(z)^{q_z}$$

$$q_R = q_1 + q_2 \times \left(\frac{d\ln\sigma}{d\ln R} + 0.5\right)$$

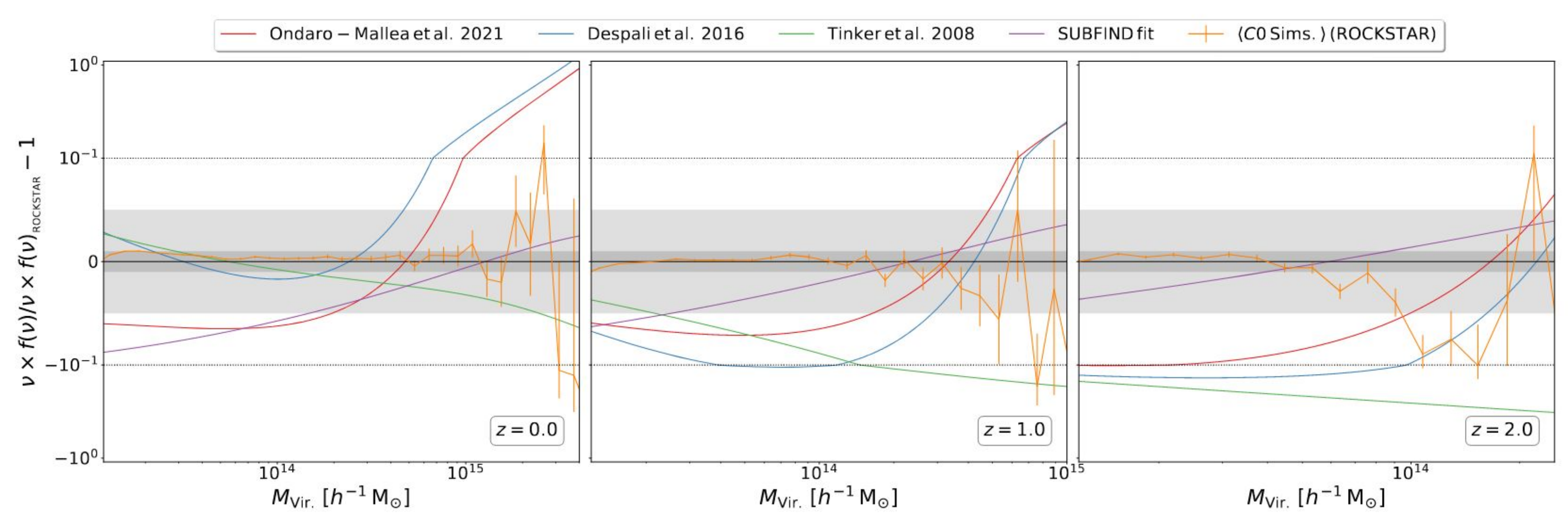
$$p = p_1 + p_2 \times \left(\frac{d\ln\sigma}{d\ln R} + 0.5\right)$$

$$a = a_R \times \Omega_m(z)^{a_z}$$

$$a_R = a_1 + a_2 \times \left(\frac{d\ln\sigma}{d\ln R} + 0.5\right)^2$$

The HMF: Non-universality modelling

- Calibration accuracy:



The HMF: Non-universality modelling

- Calibration accuracy:
  - Similar results were obtained by comparing our calibration directly with the simulations used and made available by Ondaro-Mallea et al. (2021), reassuring the robustness of our calibration.
  - 1% agreement with the Uchuu results at z=0 despite the factor of >1.000 in the computational cost of the simulations.

The DUCA suite I

Co*N*cept: Open-source *N*-body code in **!python!** public released and documented

- On-the-fly Initial Conditions: Up to third-order Lagrangian perturbation theory (3LPT).
- Hybrid Gravity Solver:
  - Particle-Mesh (PM) for long-range forces, including relativistic species perturbations under general relativity
  - Particle-Particle-Particle-Mesh (P^3M) for short-range interactions; force-split parameters adjustable per simulation
- Massive Neutrino Treatment:
  - **Linear grid-based solver for neutrino density and velocity perturbations**
  - Optional nonlinear continuity + Euler solver for neutrinos (Dakin et al. 2019b)
- **Dark Energy Perturbations: Incorporated at background and linear levels via continual grid realization**

The realization method

COSIRA (Brandbyge et al. 2017) Method Overview

1. Realize linear density field of relativistic species from a Boltzmann code power spectrum.
2. Impose Fourier phases from the existing N-body initial conditions.

$$\delta_{\rm rel}(\mathbf{k}, z) = \sqrt{P_{\rm rel}(k, z)}\ \exp\left[i\,\varphi_{\rm CDM}(\mathbf{k})\right]$$

where

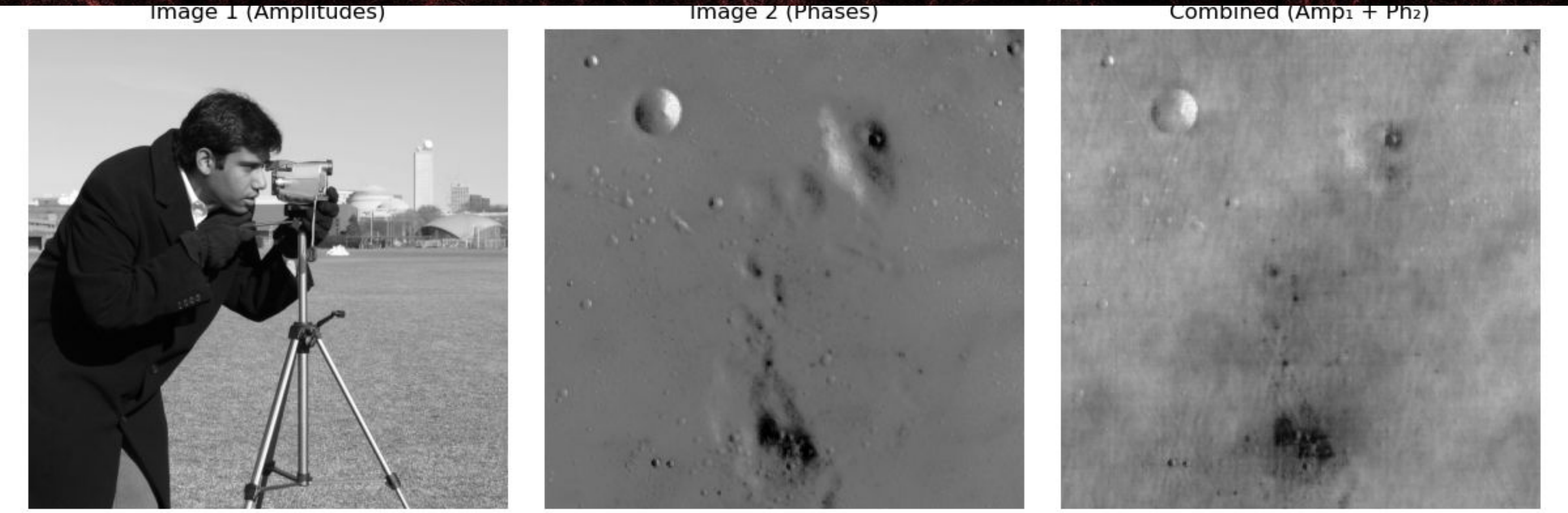
$$\varphi_{\rm CDM}(\mathbf{k})$$

are the phases from the CDM initial realization.

3. Compute potential contribution via Poisson equation and add to total.

The realization method

$$\delta_{\rm rel}(\mathbf{k}, z) = \sqrt{P_{\rm rel}(k, z)}\ \exp\left[i\,\varphi_{\rm CDM}(\mathbf{k})\right]$$



The DUCA suite I

- Key Features:
  - 3LPT initial conditions: higher-order perturbation theory allows the simulation to starts at lower redshift; minimizing transient systematics and improving efficiency.
  - Paired-Phase Technique: Amplitude fixing and π-shifted phases reduce cosmic variance in calibration runs.
  - High precision/accuracy numerical setup.
- Volume and Resolution Trade-off:
  - Large-volume runs enhance statistics of rare, high-mass halos.
  - High-resolution runs probe low-mass halos down to ~200 particles.
- Validation: Independently seeded simulations assess model predictive power.

The DUCA suite I

Table 1. Force parameters used in the DUCA set of simulations, including short-range and long-range force specifications.

Parameter	Value	Description
Short-Range Force Parameters		
`scale`	$1.25 \times$ `boxsize/gridsize`	Long/short-range force split scale
`range`	$5.5 \times$ `scale`	Maximum reach of short-range force
`tablesize`	2^{12}	Size of tabulation for short-range forces
Long-Range Force Parameters		
`gridsize_pm`	$\sqrt[3]{N}$	Particle-mesh (PM) grid size for gravity
`gridsize_p3m`	$2 \times \sqrt[3]{N}$	Particle-Particle Particle-Mesh (P3M) grid size for gravity

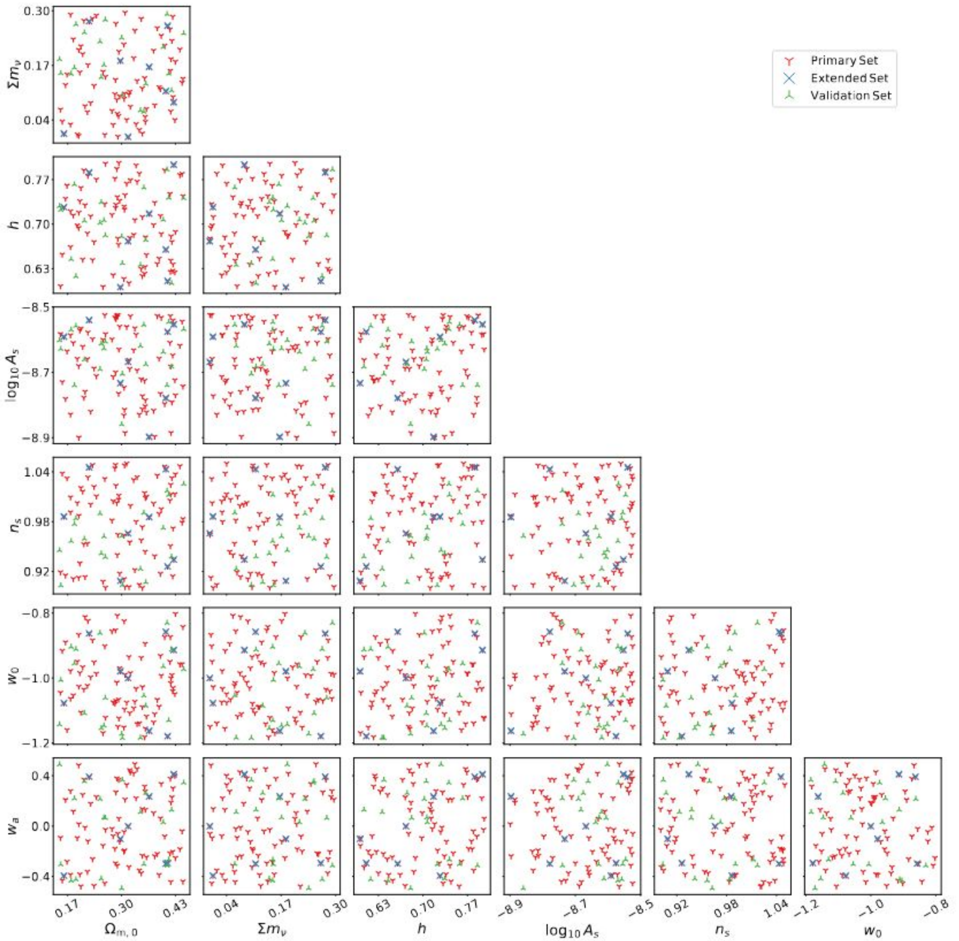
Notes. The adopted setup for the DUCA simulation set splits the long-range forces into two grids. The particle-mesh (with a grid size specified by `gridsize_pm`) is used to continually realize the massive neutrinos and DE fluctuations according to general relativity. The particle-particle-particle-mesh (with a grid size specified by `gridsize_p3m`) is used for the gravity interaction between the CDM plus baryons component. We adopted grid sizes proportional to the cubic root of the total number of particles in the simulation `N`.

Table 2. Summary of the simulation sets used in this work.

Simulation Set	Number of Sims	Box Size $[h^{-1}\mathrm{Gpc}]$	Particle Number	Mass Resolution $[(h/\Omega_{\mathrm{m},0})^{-1} M_{\odot}]$	Initial Phases	Purpose
Primary Set	82 pairs	1	1024^3	$\sim 2.6 \times 10^{11}$	Fixed and Paired	Calibration
Large Volume	8 pairs	2	2048^3	$\sim 2.6 \times 10^{11}$	Fixed and Paired	Calibration
High Resolution	8 pairs	1	2048^3	$\sim 3.2 \times 10^{10}$	Fixed and Paired	Calibration
Validation Set	20	1	1024^3	$\sim 2.6 \times 10^{11}$	Random	Validation

The DUCA suite I

Cosmological parameters



The DUCA suite II

Simulation Framework

- Volume & Resolution: 2 h^{-1} Gpc box, 2048^3 particles, initial conditions at z_{ini} = 24 via 3LPT
- Fixed cosmological parameters adopted:
  - H_0 = 67 km s^{-1} Mpc^{-1}
  - $\Omega_{b,0}$ = 0.049
  - $\Omega_{cdm,0}$ = 0.27
  - $A_s = 2.1 \times 10^{-9}$
  - n_s = 0.96
  - Massless neutrinos

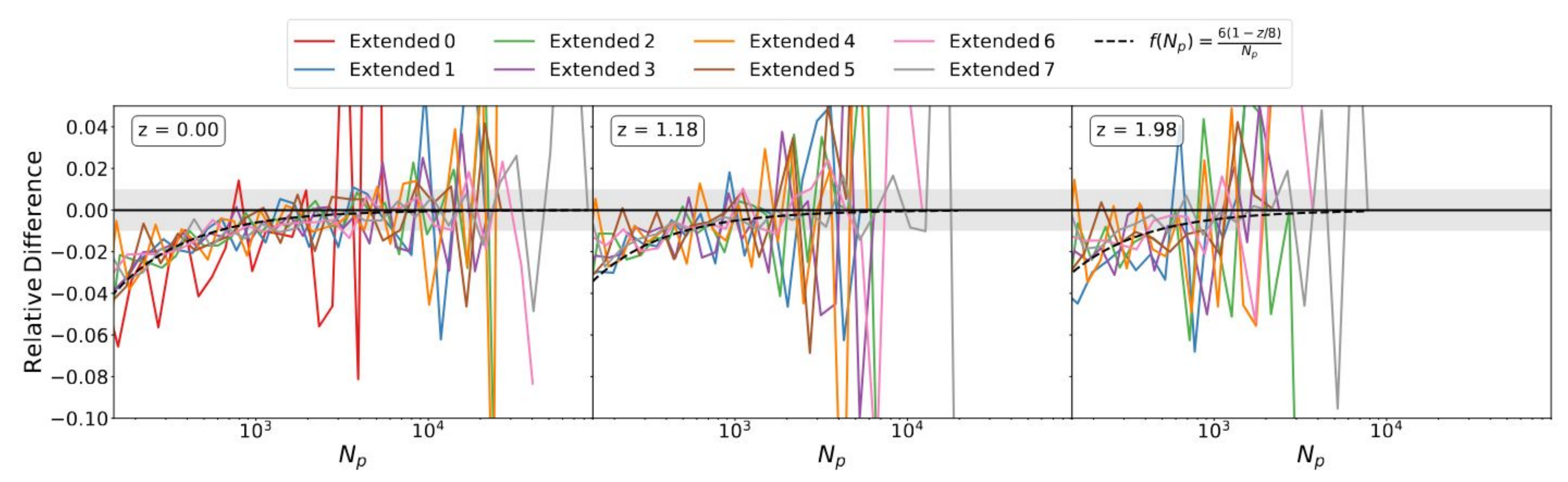
Table 1. DE parameter combinations for the simulation suite.

Simulation #	c_s^2	w_0	w_a	PPF	Fluid	Phantom Twin
1	10^{-7}	−1.0	0.3	✓	✗	✗
2	10^{-7}	−0.9	0.2	✓	✗	✗
3	10^{-7}	−0.8	0.1	✓	✓	✓
4	10^{-5}	−1.0	0.3	✓	✗	✗
5	10^{-5}	−0.9	0.2	✓	✗	✗
6	10^{-5}	−0.8	0.1	✓	✗	✗
7	10^{-3}	−1.0	0.3	✓	✗	✗
8	10^{-3}	−0.9	0.2	✓	✗	✗
9	10^{-3}	−0.8	0.1	✓	✗	✗
10	1	−1.0	0.3	✓	✗	✗
11	1	−0.9	0.2	✓	✓	✓
12	1	−0.8	0.1	✓	✗	✗

Modelling the cluster counts in collisionless simulations

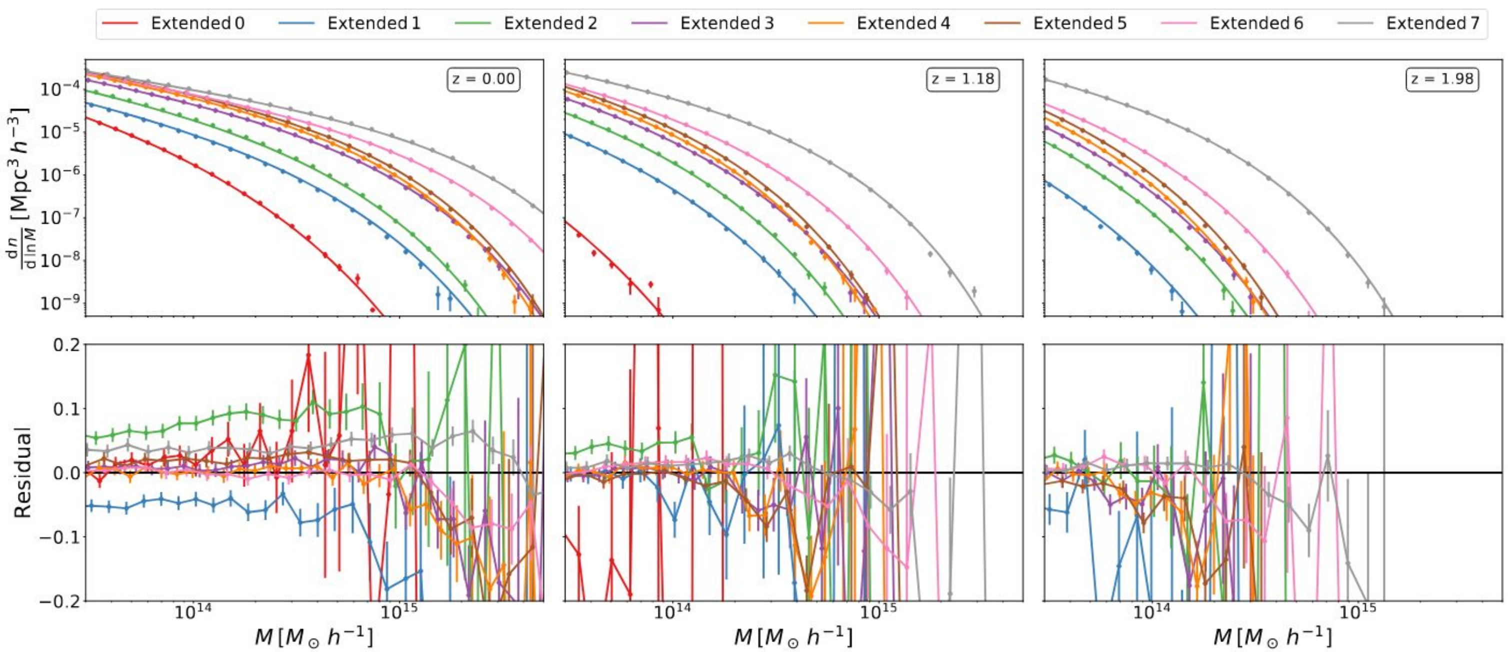
DUCA I: The HMF in dynamical dark energy cosmologies

Impact of mass resolution:



DUCA I: The HMF in dynamical dark energy cosmologies

Comparison with the LCDM model:



DUCA I: The HMF in dynamical dark energy cosmologies

Multiplicity Function

$$\nu\, f(\nu) = 2\,A \left\{ \nu_*^r + \left(\frac{\nu_p}{\nu_*}\right)^{2p} \right\} \frac{\nu_*}{\sqrt{2\pi}} \exp\!\left(-\frac{\nu_*^2}{2}\right) \nu_*^{q-1}$$

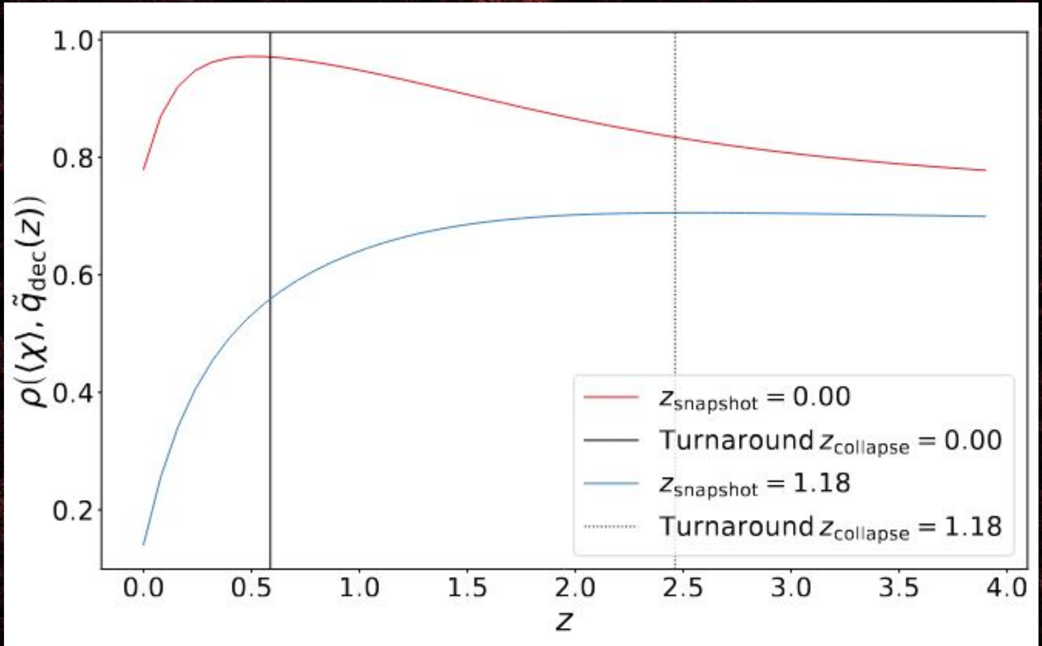
where

$$A \text{ set by } \int f(\nu)\, d\ln\nu = 1.$$

$$\nu = \frac{\delta_c}{\sigma(M,z)}, \quad \nu_* = \sqrt{a}\,\nu,$$

DUCA I: The HMF in dynamical dark energy cosmologies

Comparison with the LCDM model:



DUCA I: The HMF in dynamical dark energy cosmologies

Parameter Evolution with Dynamical Dark Energy

$$x_i = x_{\Lambda,i}\left[1 + \widetilde{q}_{\rm dec}(z_{\rm ta};\alpha_i,\beta_i)\right]$$

$$\widetilde{q}_{\rm dec}(z_{\rm ta};\alpha,\beta) = \frac{3\alpha}{2}\left[w_{\rm DE}(z_{\rm ta})+1\right]\Omega_{\rm DE}(z_{\rm ta})^{\beta}$$

with turnaround redshift

$$1 + z_{\rm ta} = (1+z)\,2^{-2/3} \quad\Longrightarrow\quad z_{\rm ta} = \frac{1+z}{2^{2/3}} - 1.$$

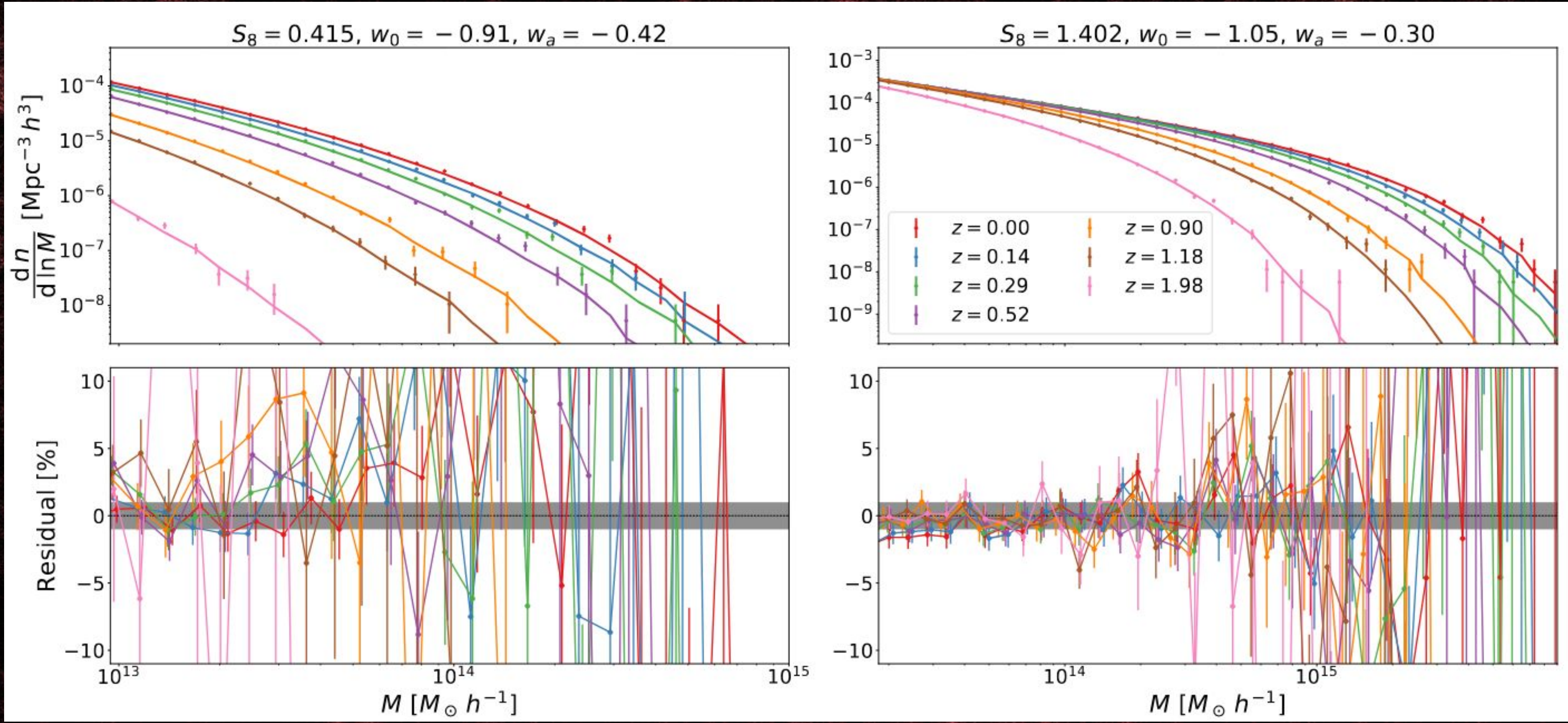
Key Points

– The extra exponent r and pivot vp allow a double power–law form.

– Dark energy enters through the deceleration parameter evaluated at collapse turnaround.

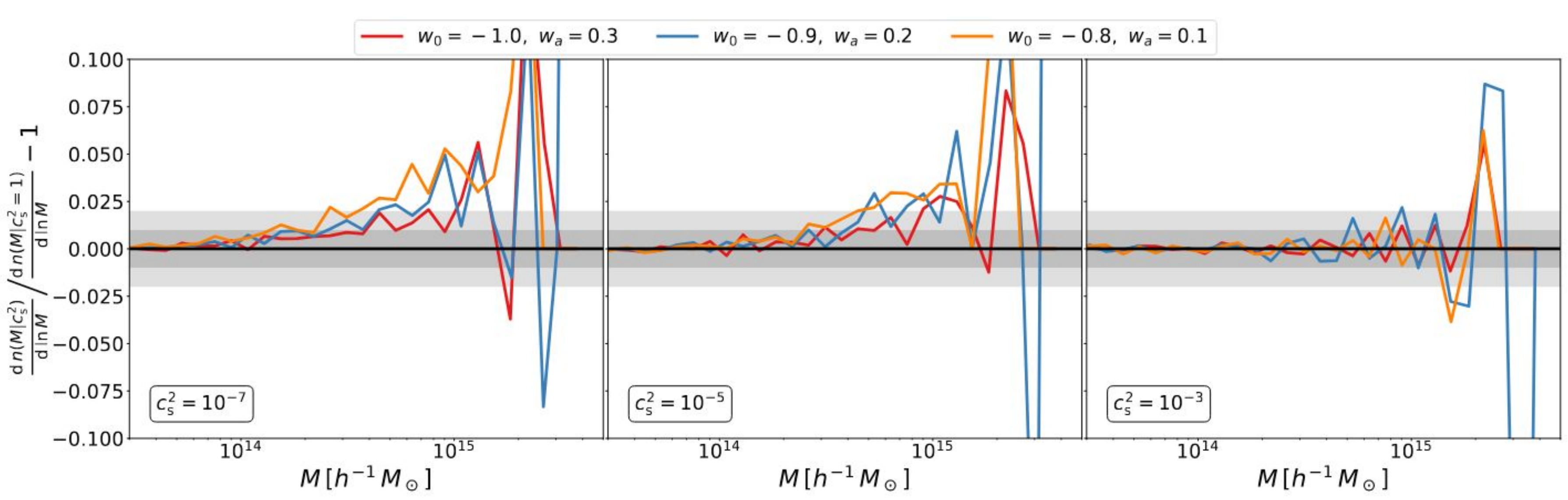
– Achieves sub-percent accuracy over wide (w0,wa) space.

DUCA I: The HMF in dynamical dark energy cosmologies



DUCA II: The HMF in clustering dark energy cosmologies

Comparison with “non-clustering” case (simulation only):



DUCA II: The HMF in clustering dark energy cosmologies

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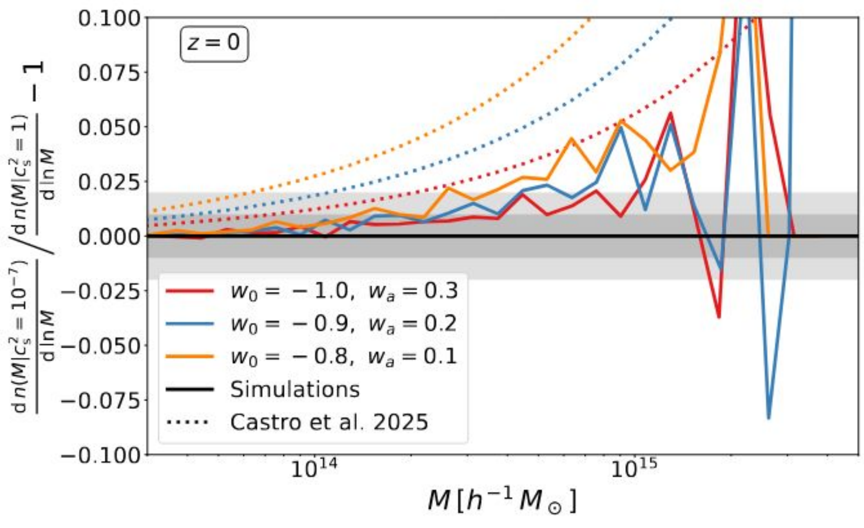
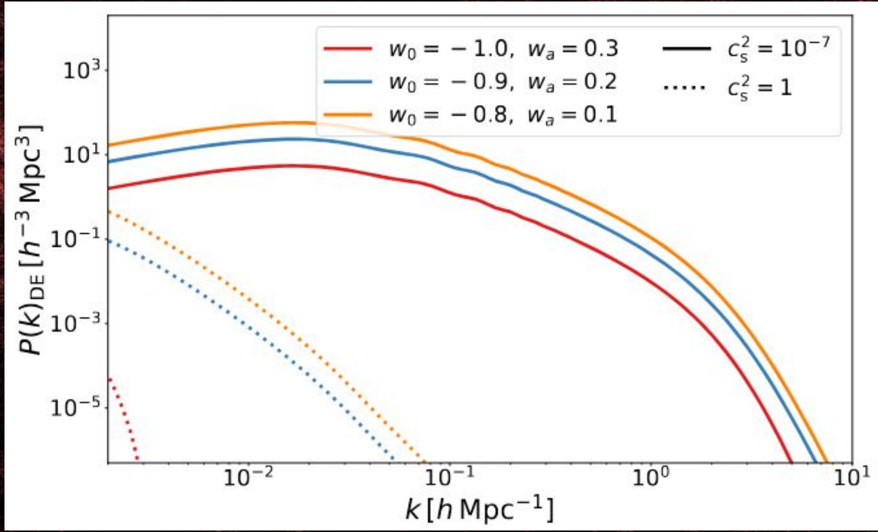




DUCA II: The HMF in clustering dark energy cosmologies

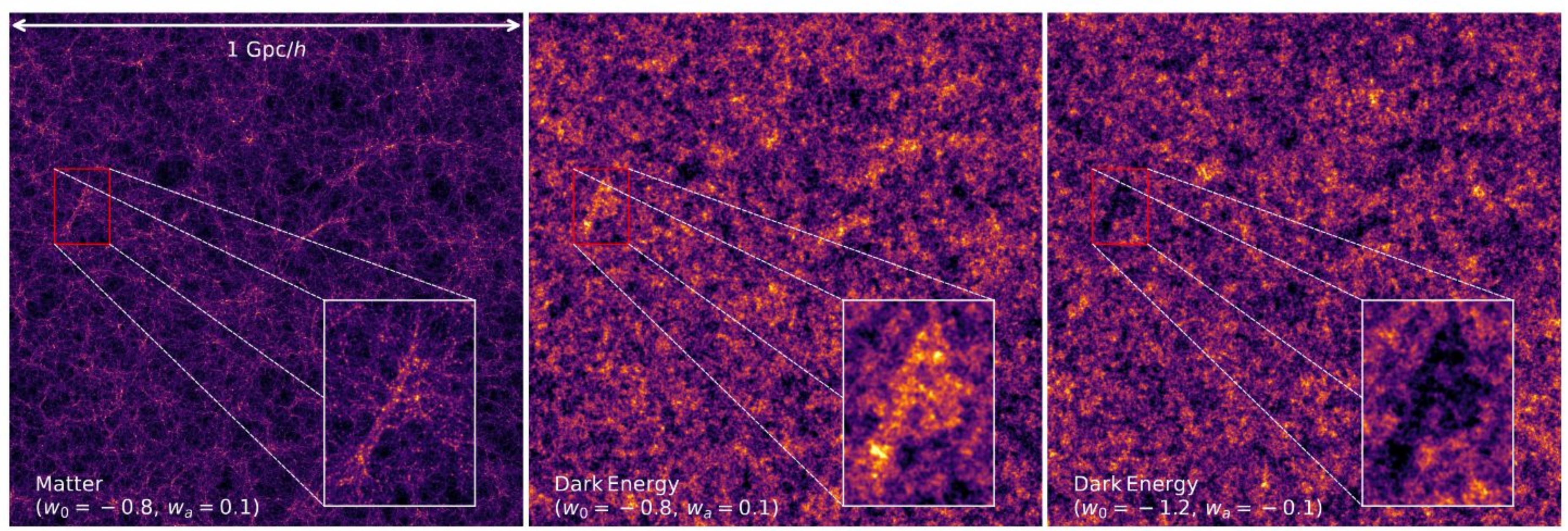
Effective Peak-Height Modification:

$$\nu_{\rm eff}(M, z \mid c_s < 1) = \frac{\nu(M, z \mid c_s = 1)}{1 + \lambda\, \mathrm{sgn}\big[1 + w(z_{\rm ta})\big] \frac{\Omega_{\rm DE}(z_{\rm ta})\, \sigma_{\rm DE}(R_{\rm ta}, z_{\rm ta})}{\Omega_m(z_{\rm ta})\, \sigma_m(R, z_{\rm ta})} \frac{\delta_{\rm ta}^{\rm EdS}}{\Delta_{\rm ta}^{\rm EdS}}}$$

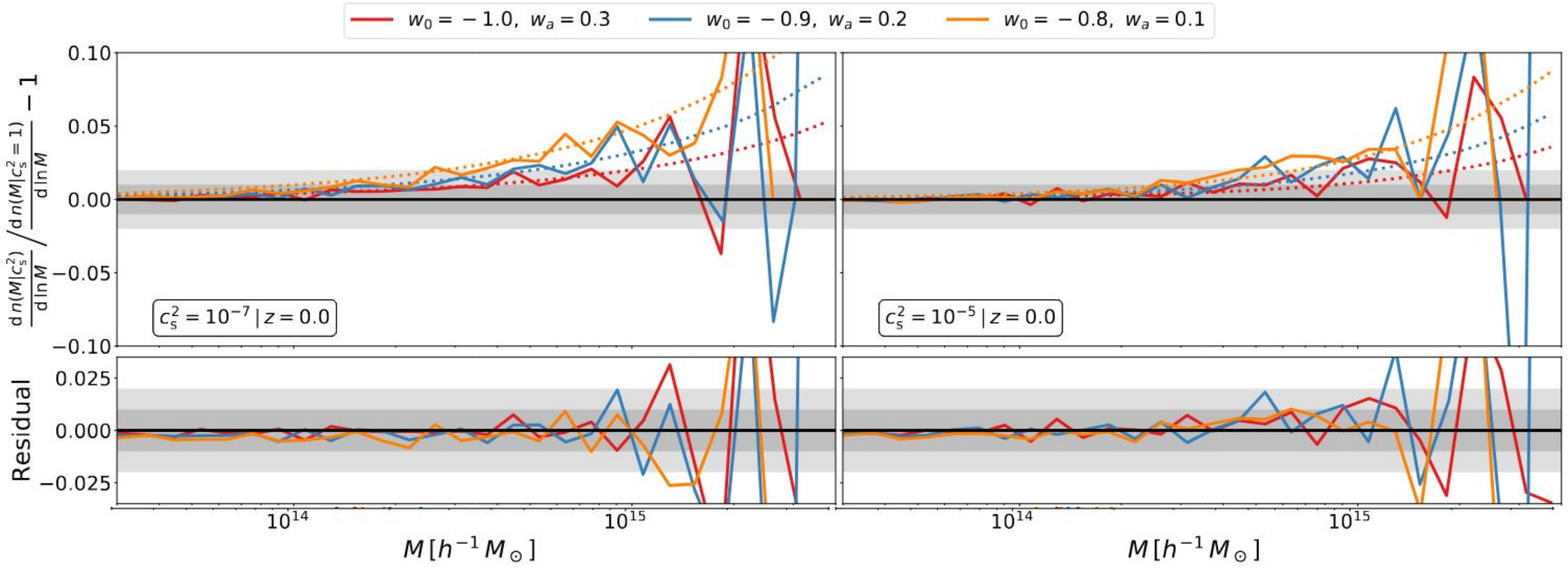
Key Points:

1. Introduces single calibration constant λ (best-fit ~ 0.34).
2. Accounts for reduced DE clustering relative to matter via variance ratio at turnaround.
3. Recovers baseline model when cs→1 (σDE→0).
4. Achieves sub-percent accuracy across cs values.

DUCA II: The HMF in clustering dark energy cosmologies

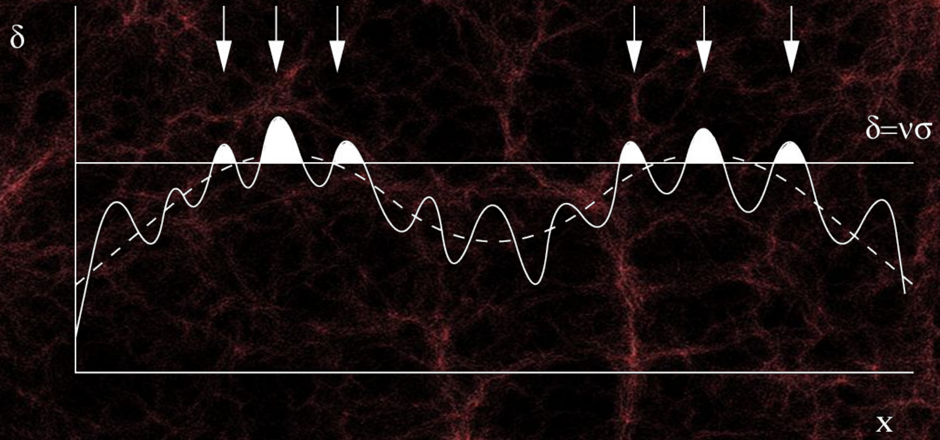


DUCA II: The HMF in clustering dark energy cosmologies



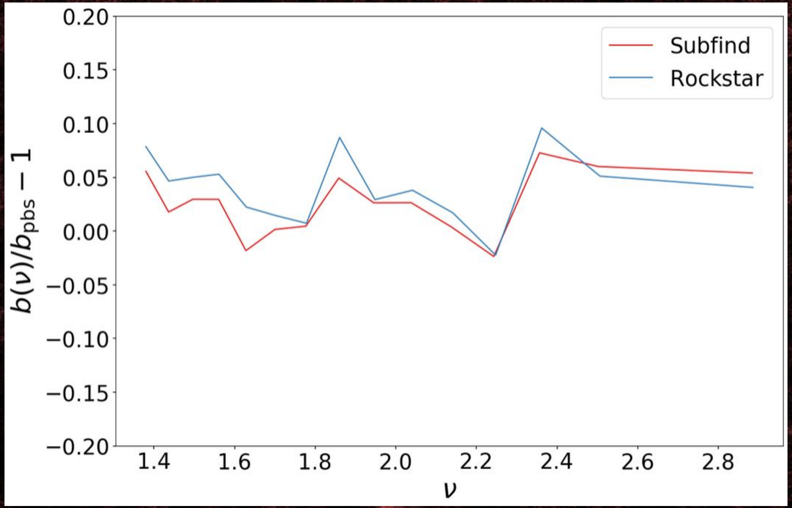
Modelling the cluster clustering in collisionless simulations

The halo bias: Peak-background split



1. **Press-Schechter formalism**:
   - Fraction of matter in halos:
     - $\frac{dn(M,z)}{dM} = \frac{\rho_{mc} dP(\delta M/\sigma(M,z)>\nu)}{M dv}$
2. **Multiplicity function**:
   - As probability:
     - $f(M,z) = \frac{dP}{d\nu} = \frac{dP}{dM}$
3. **Peak-Background Split**:
   - Linearly evolved matter density:
     - $\delta(x)$ split into short (δ_s) and long (δ_l) correlation lengths.
   - Condition:
     - $P(\delta M/\sigma > \nu | x) \approx P(\delta M/\sigma > \nu - \delta M(x)/\sigma)$
4. **Halo density contrast**:
   - Defined as:
     - $\delta_h(M,z,x) = \frac{n(M,z,x)}{n(M,z)} - 1 = \frac{-1}{\sigma(M,z)} \frac{d \log f}{d\nu} \delta M(z,x)$
5. **Halo bias on Lagrangian space**:
   - Transition to σ:
     - $b_L = -\frac{\delta_c(z) d \log f(z,\sigma)}{d\sigma}$
   - Eulerian space:
     - $b = b_L + 1$

The halo bias: Peak-background split



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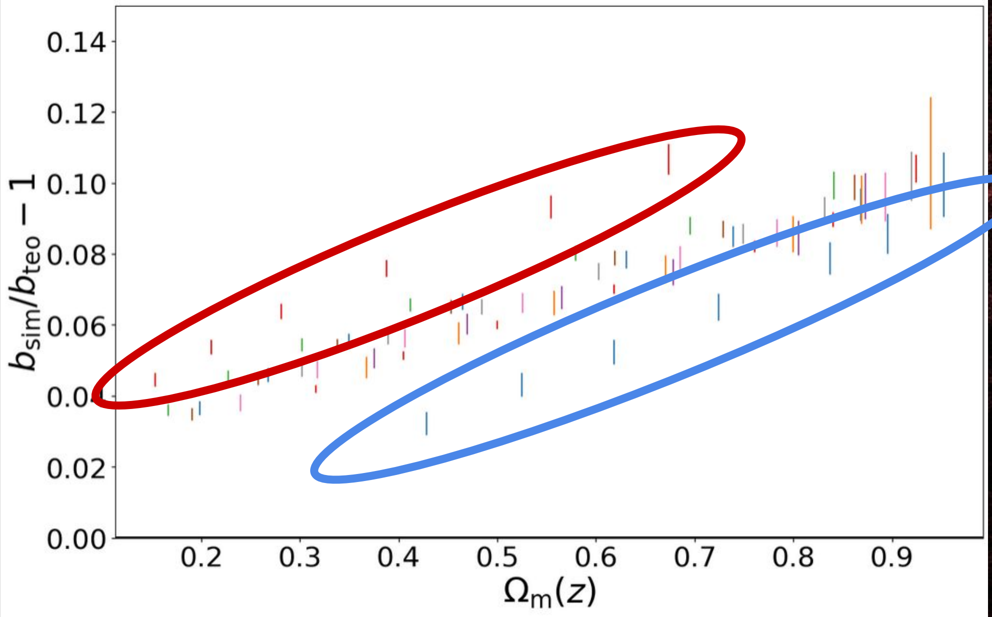
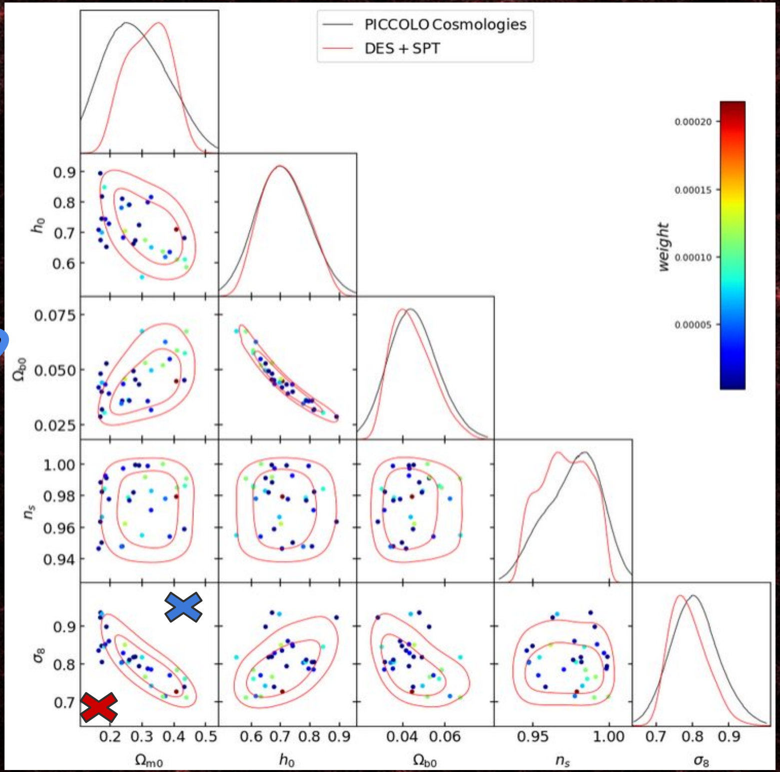
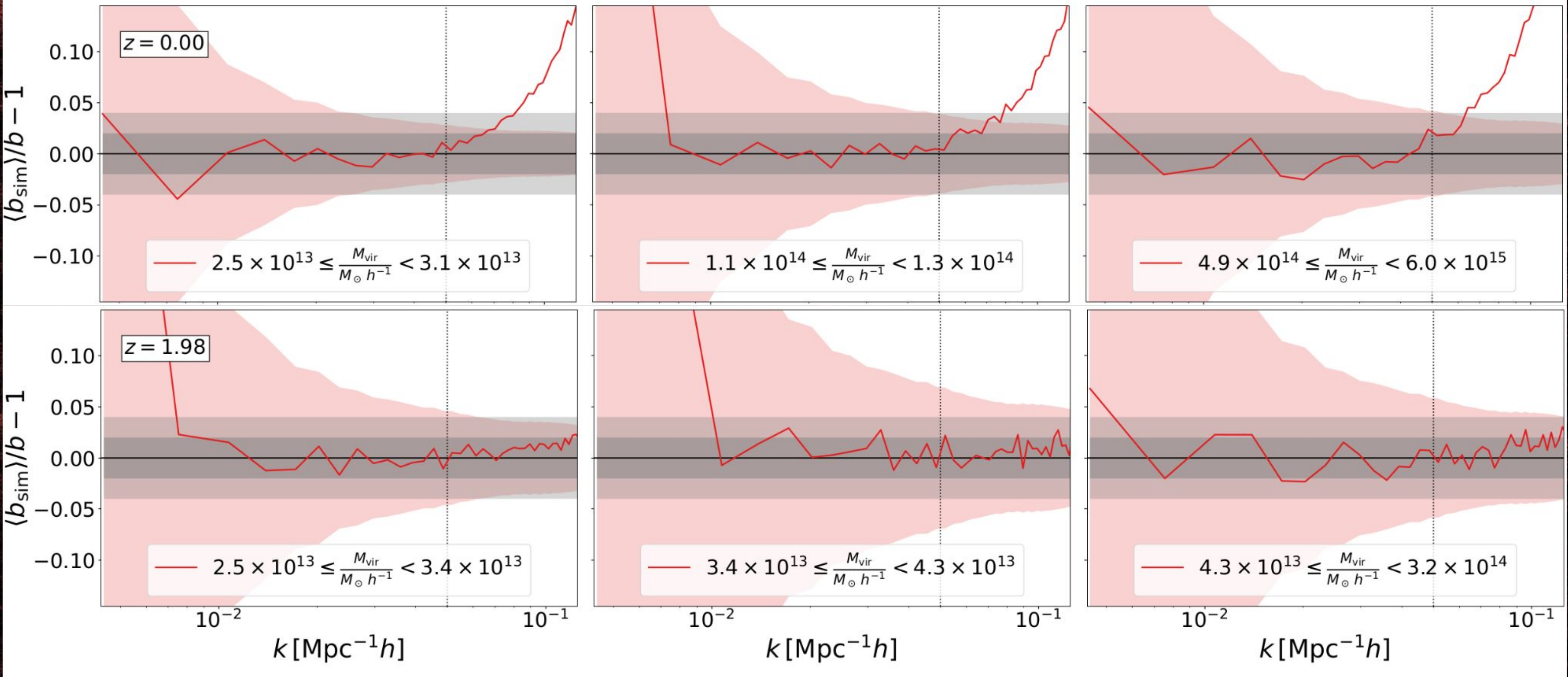
The halo bias: Peak-background split bias

- Modelling the PBS correction:





The halo linear bias:



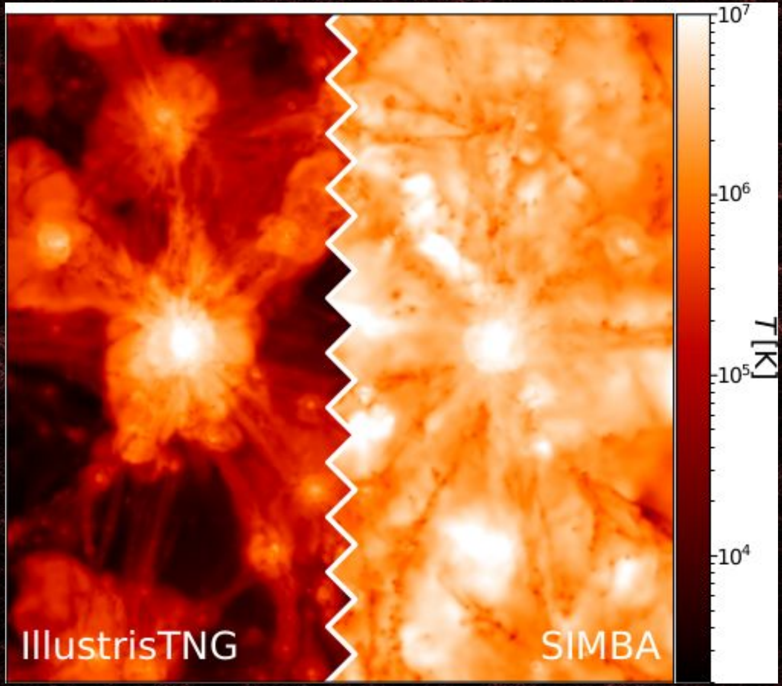
Modelling the impact of baryons on clusters

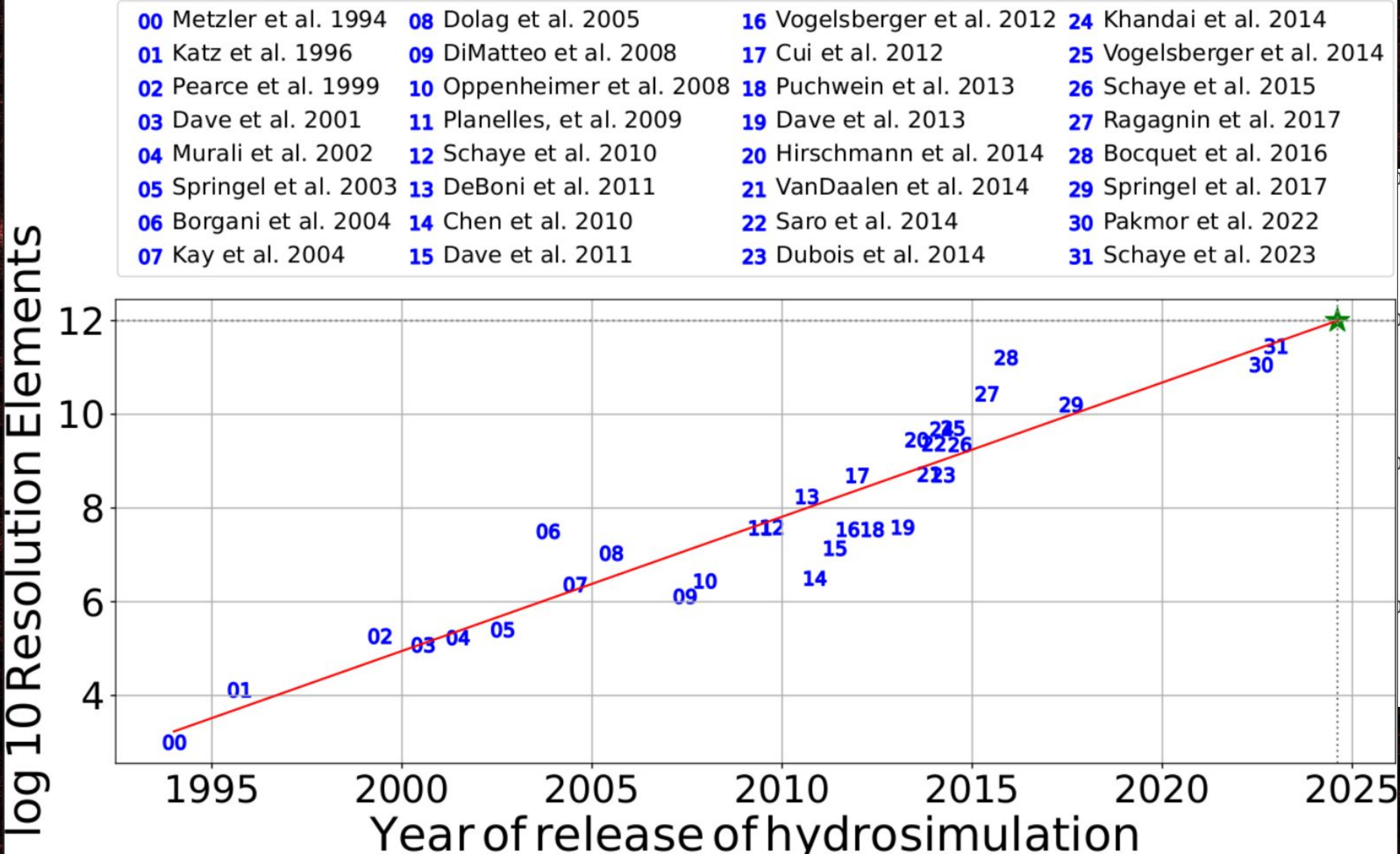
Methodologies Used for Modeling Baryonic Feedback

1. Overlooking Baryonic Impact	This approach, increasingly viewed as outdated, poses a risk of misinterpreting high-quality cosmological data.
2. Discarding Dominant Baryonic Regimes	Although initially logical, this strategy is limited by the universe's complex and overlapping zones of influence (see, for instance, Martinet et al., 2021).
3. Relying on a Fiducial Hydro Simulation	While common, the overarching nature of this method may not adequately represent the diversity of baryonic interactions (see, for instance, Harnois-Deraps et al., 2021; Heydenreich et al., 2022; Burger et al., 2023a,b)
4. Adopting Machine Learning as a black box	Despite its advanced nature, it brings computational intensity challenges and potential baryonic physics obfuscation (see, for instance, Shao et al., 2023a,b; de Santi et al., 2023)

Sub-resolution calibration:

- The free parameters in the sub-resolution modelling has to be carefully adjusted in order to produce reasonably reliable results.
- There is no cartesian set of observables that by reproducing them a hydro simulation is validated.
- The cost of hydro simulations forbids common bayesian methods to be used for the calibration of the sub-resolution modeling
- **These complexities results on a perplexing difference between state-of-the-art hydro simulations.**




00 Metzler et al. 1994
01 Katz et al. 1996
02 Pearce et al. 1999
03 Dave et al. 2001
04 Murali et al. 2002
05 Springel et al. 2003
06 Borgani et al. 2004
07 Kay et al. 2004
08 Dolag et al. 2005
09 DiMatteo et al. 2008
10 Oppenheimer et al. 2008
11 Planelles, et al. 2009
12 Schaye et al. 2010
13 DeBoni et al. 2011
14 Chen et al. 2010
15 Dave et al. 2011
16 Vogelsberger et al. 2012
17 Cui et al. 2012
18 Puchwein et al. 2013
19 Dave et al. 2013
20 Hirschmann et al. 2014
21 VanDaalen et al. 2014
22 Saro et al. 2014
23 Dubois et al. 2014
24 Khandai et al. 2014
25 Vogelsberger et al. 2014
26 Schaye et al. 2015
27 Ragagnin et al. 2017
28 Bocquet et al. 2016
29 Springel et al. 2017
30 Pakmor et al. 2022
31 Schaye et al. 2023
log 10 Resolution Elements
Year of release of hydrosimulation
T[K]

A Novel Model to Quantify Baryonic Impact: UPSHIFT

1. Data-driven

Due to the inherent limitations in simulating baryonic feedback from first principles,only a robust data-driven methodology ensure that predictions remain aligned with observations.

2. Universality

An ideal model for baryonic effects should not be limited to mimic hydro simulations, but offer a transversal and universal description.

3. Validation

A model can only be validated if realistic estimations of the uncertainties involved follow predictions.

Understanding the Baryonic feedback within Clusters

- Impact on Euclid Cluster Cosmology:
  - Ignoring the impact of baryons might significantly bias the cosmological constraints
  - Limiting to more massive, less affected clusters affects the FOM by an order of magnitude
  - Modeling the impact of baryons on cluster masses gives the optimal trade-off.

Table 7. FoM in units of 10^3 and Index of Inconsistency (IOI) in σ units (Lin & Ishak 2017), without and with corrections for mass variations.

S/N of Euclid forecast	3	5
FoM (Hydro)	137	19.4
FoM (DMO)	114	17.0
$\sqrt{2\mathrm{IOI}}$ DMO wrt Hydro	8.1	1.1
FoM (DMO+Hydro correction)	120	15.6
$\sqrt{2\mathrm{IOI}}$ Corrected DMO wrt hydro	1.1	1.0

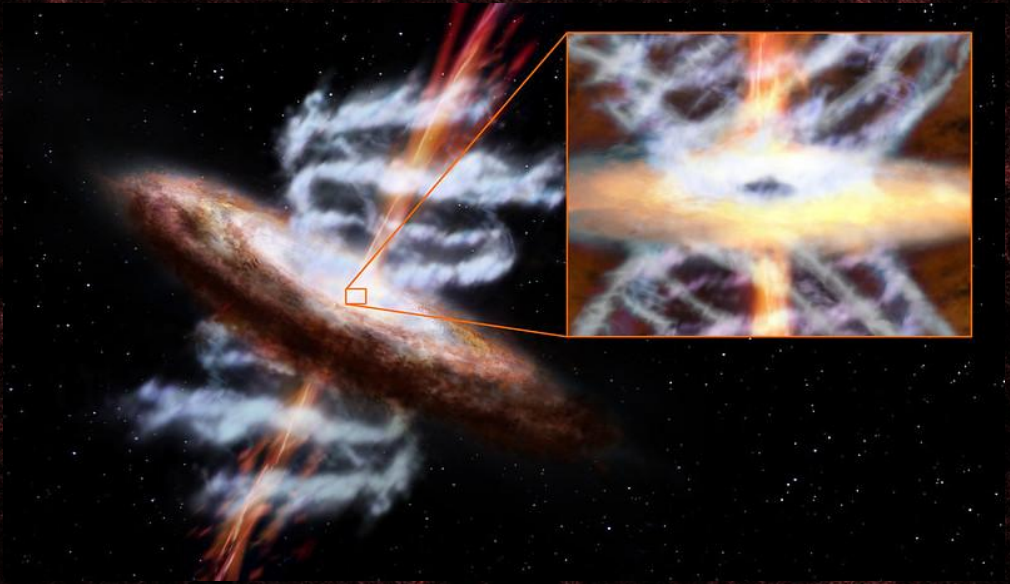
Effect of Baryons

MAGNETICUM

- Magneticum takes into account:
  - Cooling, star formation, winds (Springel & Hernquist 2003);
  - Metals, stellar population and chemical enrichment;
  - SN-Ia, SN-II, AGB (Tornatore et al. 2003/2006);
  - BH and AGN feedback (Springel & Di Matteo 2006, Fabjan et al. 2010);
  - Thermal Conduction (1/20th Spitzer) (Dolag et al. 2004);
  - Low viscosity scheme to track turbulence (Dolag et al. 2005);
  - Higher order SPH Kernels (Dehnen & Aly 2012);
  - Magnetic Fields (passive) (Dolag & Stasyszyn 2009).

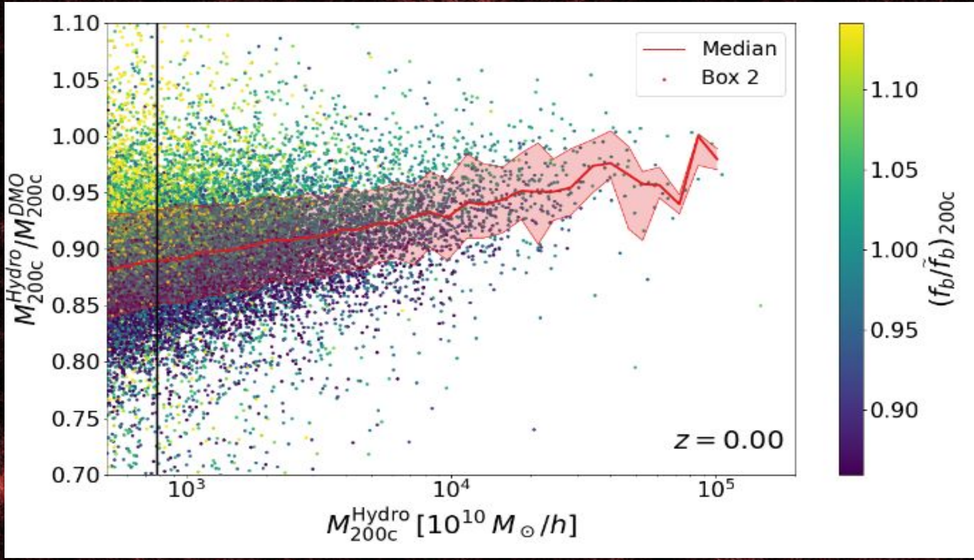
The HMF: Effect of Baryons

- A more consistent picture of AGN feedback:



The HMF: Effect of Baryons

- Baryons affect the LSS:
  - **The net effect is that matched halos has systematically lower masses on hydro than on the DMO;**
  - Cluster abundance is suppressed by 5-15%;



The HMF: Effect of Baryons

- Baryonic feedback impact on halo masses:
  - Quasi-adiabatic model:

$$M_{\Delta,\mathrm{dmo}} R_{\Delta,\mathrm{dmo}} = M_{\mathrm{vir,hyd}} R_{\mathrm{vir,hyd}}$$

$$M_{\Delta,\mathrm{dmo}} = \frac{1 - f_{\mathrm{b,vir}}}{1 - f_{\mathrm{b,cosmic}}} M_{\mathrm{vir,hyd}}$$

$$\Delta = \frac{3\, M_{\Delta,\mathrm{dmo}}}{4\pi R^3_{\Delta,\mathrm{dmo}} \rho_c} \,,$$

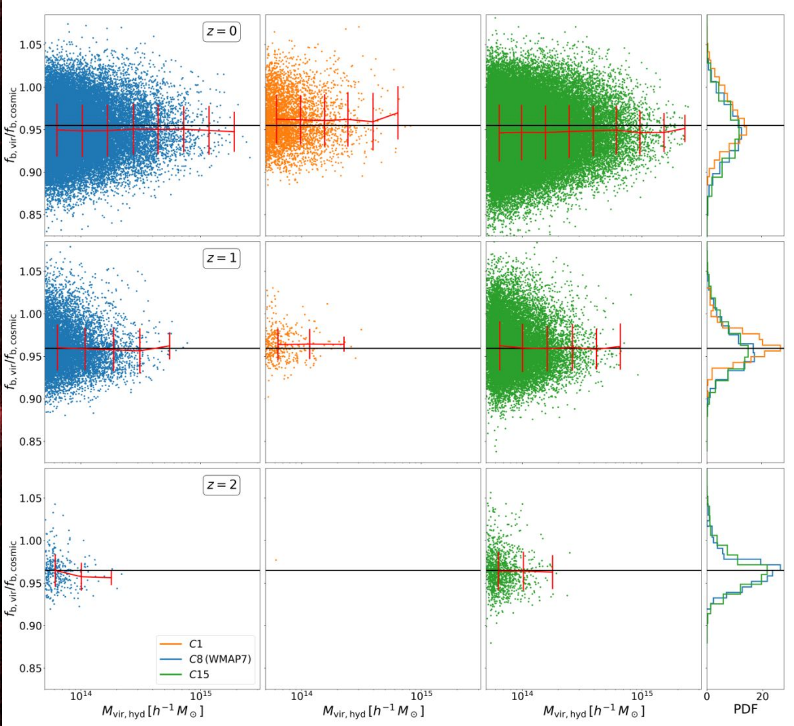
"I think nature's imagination is so much greater than man's, she's never going to let us relax."
R. Feynman

$$M_{\Delta,\mathrm{dmo}} = \frac{1 - f_{\mathrm{b,vir}} - \delta_f}{1 - f_{\mathrm{b,cosmic}}} M_{\mathrm{vir,hyd}} \,,$$

$$\frac{R_{\Delta,\mathrm{dmo}}}{R_{\mathrm{vir,hyd}}} = 1 + q \left(\frac{1 - f_{\mathrm{b,cosmic}}}{1 - f_{\mathrm{b,vir}} - \delta_f} - 1 \right)$$

Calibration of the quasi-adiabatic model

- **Calibration of the δf parameter:**
  - **For the calibration of the baryonic offset (δ f), we concentrate on the non-radiative versions of the Magneticum Box 1a.**
  - **These simulations serve as a fundamental calibration point for the baryon fraction, providing a baseline scenario wherein the other effects are assumed to balance to zero.**
  - **Even without feedback, cluster sized halos do not lock the cosmic baryon fraction, instead they contain around 95% of it.**
  - **Even not locking the entire baryon fraction, there is no statistical difference in the masses between the NR and DMO objects.**



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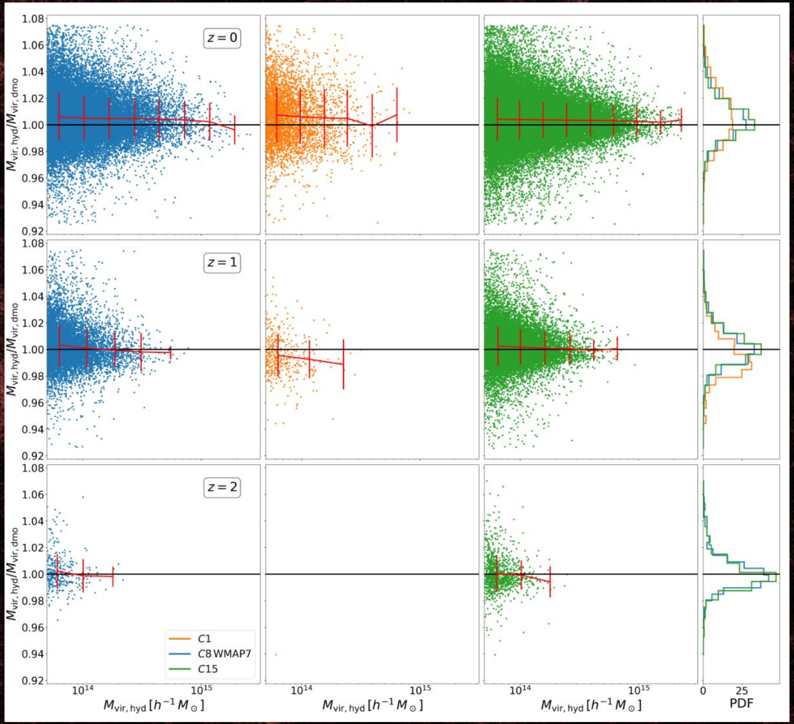
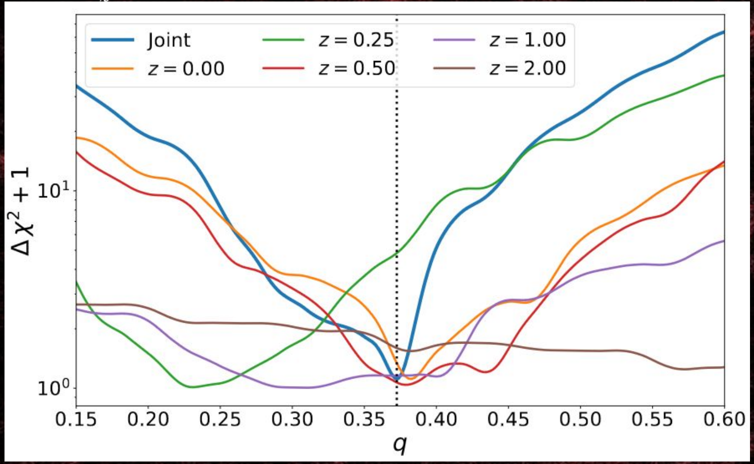


Calibration of the quasi-adiabatic model

Calibration of the q parameter:

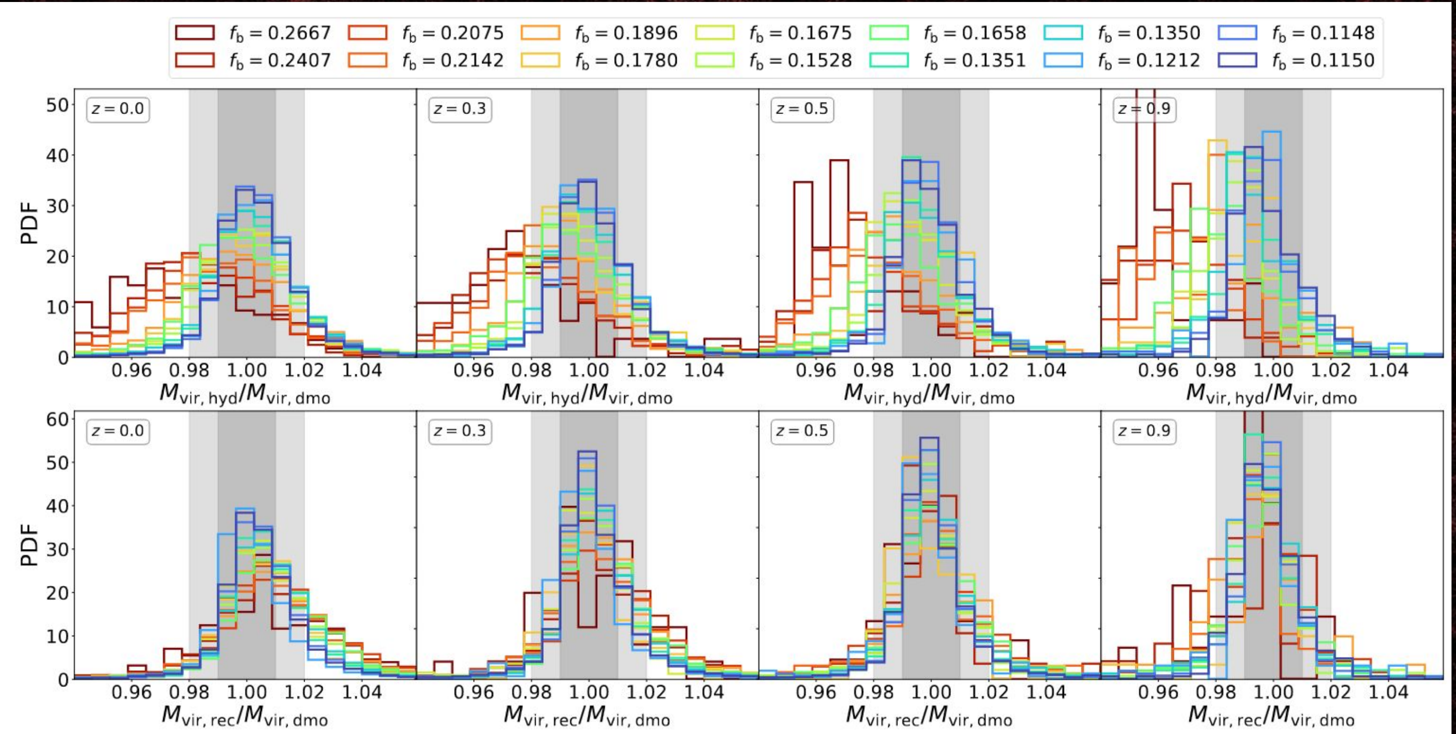
- **For the calibration of the quasi-adiabatic parameter (q), the Magneticum hydrodynamic Box 2 simulations are utilized. This introduces a more advanced level of simulation complexity, building upon the foundational understanding established through the calibration of δ f .**

$$\chi^2 = \sum_{i,j} \left(\frac{\langle M_{vir,rec}/M_{vir,dmo} \rangle - \langle M_{vir,hyd}/M_{vir,dmo} \rangle}{\sigma_{i,j}} \right)^2_{i,j}$$



The HMF: Effect of Baryons

- Stressing the model…



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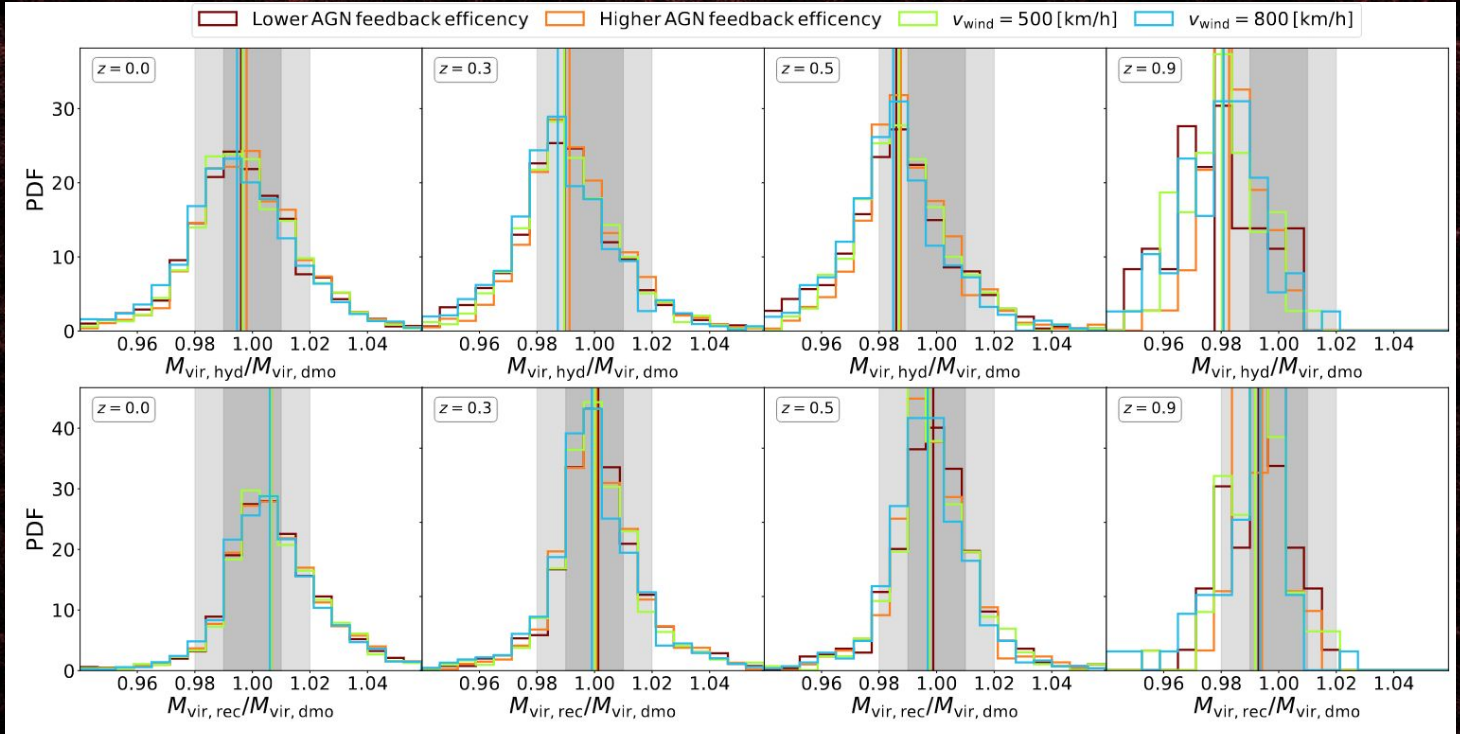

The HMF: Effect of Baryons

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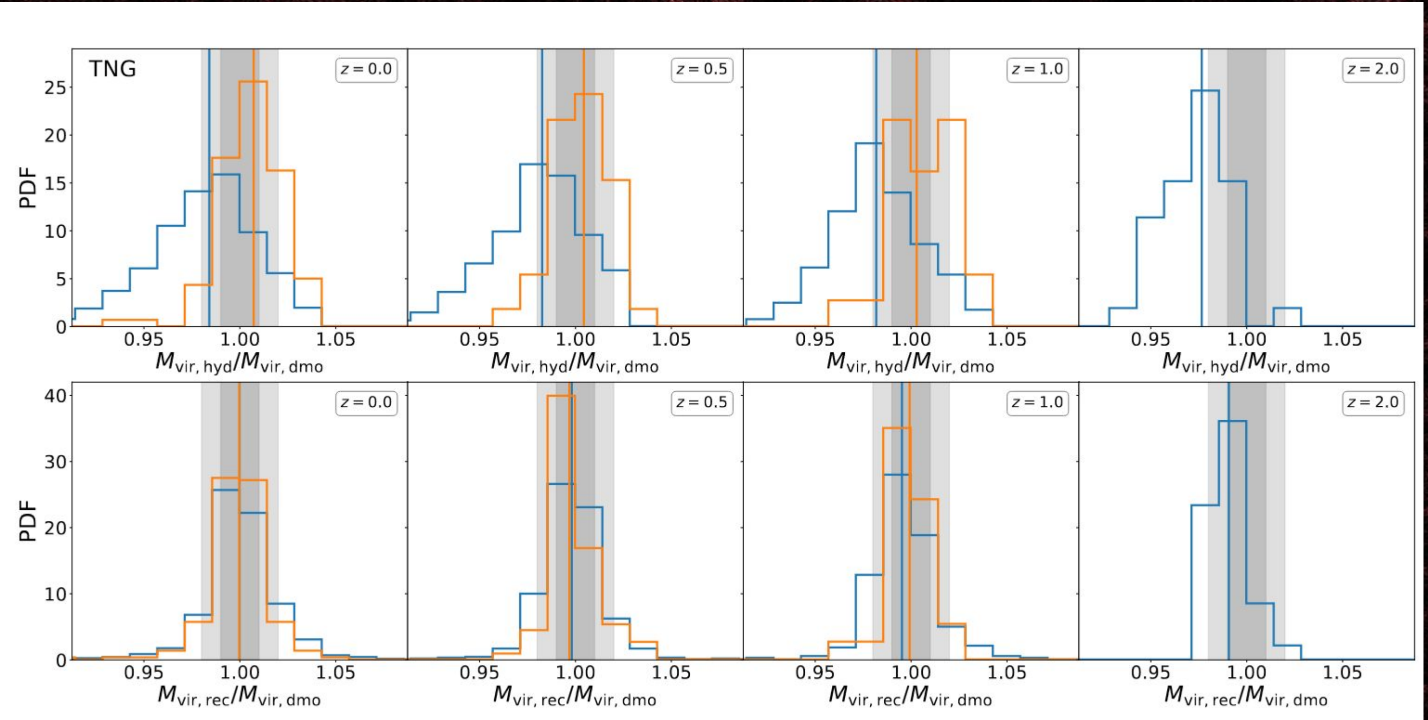

Conclusions

1. In Euclid Collaboration: Castro et al. 2023a, we introduce a calibrated analytical HMF, ensuring its accuracy to make it less uncertain in deducing cosmological parameters from Euclid cluster counts.
    a. The calibration is based on a set of N-body simulations and considers various factors like simulation methods, halo-finding algorithms, and cosmological conditions.
    b. Our final fitting function for HMF is found to be very accurate across several ΛCDM model variations, with most uncertainties being minor, except for potential biases introduced by the halo finder.

2. In Euclid Collaboration: Castro et al., 2024a, we present a calibration for the halo bias.
    a. The model uses the peak-background split (PBS) as a starting point and model how the accuracy of the PBS depends on cosmology.

3. In Euclid Collaboration: Castro et al. 2024b, we introduce a model to quantify baryons' impact on galaxy cluster halo masses.
    a. The model presents a 1% accuracy in determining virial dark matter-only cluster mass
    b. The paper also emphasizes the significance of considering baryonic effects in cosmological studies, especially for the Euclid survey, where such effects, if ignored, could bias results.

Conclusions

1. Dynamical Dark Energy (w_0,w_a evolution):
    a. Redshift-dependent corrections via the relative deceleration parameter
    b. Alters the shape of vf(v): extra degree of freedom r and pivot vp enable double power-law behaviour.
    c. Achieves sub-percent accuracy across wide (w0,wa)(w0,wa) grid, ensuring robust emulation of summary statistics.
2. Clustering Dark Energy (c□<1 regimes)
    a. Effective peak height calibrates the impact of DE clustering on halo collapse
    b. Recovers standard HMF as cs→1; delivers per-cent precision over cs values.
3. Combined Implications
    a. Both dynamic evolution and DE clustering imprint mass- and redshift-dependent deviations on the HMF at the few-percent level.
    b. Accurate modelling of next-generation surveys demands inclusion of both effects for precision cosmology.

Thanks / Grazie / Obrigado!