CONSTRAINED COSMOLOGICAL SIMULATIONS **APPLIED TO HIGH-Z SPECTROSCOPIC SURVEYS**

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"FROM GALAXIES TO COSMOLOGY WITH DEEP SPECTROSCOPIC SURVEYS", 2022 JULY 6







GALAXIES AS TRACERS OF LARGE-SCALE STRUCTURE

- Galaxies coalesce from the largescale structure that manifests into a 'cosmic web' at ~Mpc scales
- The large-scale structure is a successful prediction of ACDM cosmology
- Question: How does the cosmic web influence galaxy formation and evolution across cosmic time?





CONSTRAINED SIMULATIONS

- tracers after forward modelling (typically using semi-numerical techniques, e.g. 2LPT)
 - web emerged
- Derived initial conditions can then be used to seed N-body simulations (or even hydro!)



Density reconstruction: Construct the initial conditions so that matter density field is consistent with the distribution of

• Initial conditions: (nearly) Gaussian random fields at high redshifts (z~100) from which the large-scale structures/cosmic

• Uncertainties (data & theoretical model) lead to an ensemble of correlated realisations that are consistent with the data

• Application to SDSS Main Galaxy Survey (z~0.1) in the ELUCID Project (Wang+2014, 2016). See also HeB+2013 (2MASS)

Reconstructed Density N-body Sim



APPLICATION TO HIGH REDSHIFT GALAXY SURVEYS?

- Local Universe and near field galaxy surveys conducted with great success over the last 2 decades (2MRS, 6dFGS, GAMA, BOSS...)
- Next generation surveys (PFS, MOONS...) will cover high redshifts (z>1) with similar fidelity as the previous generations of low-redshift surveys
- Some advantages to applying constrained realization techniques to high redshift:
 - Gravitational evolution is still only mildly non-linear at z>1.5: shell-crossing has generally yet to occur
 - Directly provides matter density field as galaxy environment measure, with the observational selection function already applied
 - Can say interesting things about the growth of galaxy protoclusters into virialized clusters



THE COSMOS FIELD

- COSMOS Survey (Capak+2007; Laigle+2016...)
- Photometric survey (1 < z < 6) with 5×10^5 galaxies
- Covers the peak of star formation
- Ideal redshift range to to probe the cosmic web with "protoclusters"
- One of the most extensive spectroscopic campaigns in any high redshift deep field
- Angular footprint (~1 sq deg) also gives it sufficient transverse coverage (~100 cMpc @ z=2.5) to probe protoclusters scale (>20-30 cMpc)







PART I: DENSITY RECONSTRUCTION WITH "COSMIC-BIRTH" Ata et al 2021, MNRAS, 500, 3, 3194

- Mapping initial (Lagrangian) q to final displacement field $x = \Psi(q) + q$
- \mathcal{Y}(q) is given by the forward model

 (X-LPT, Nbody solver, particle mesh...)
 and is a function of the initial field
 (e.g. Zel'dovich Approx.

 $\boldsymbol{\Psi} = \frac{d^3k}{(2\pi)^{3/2}} e^{i\boldsymbol{k}\cdot\boldsymbol{q}} \frac{i\boldsymbol{k}}{k^2} \hat{\delta}(\boldsymbol{k})$

• We need to solve this problem iteratively

• Mapping initial (Lagrangian) q to final (Eulerian) x positions using the cosmological



COSMIC BIRTH

- COSMIC BIRTH algorithm (Kitaura, Ata+2021, arXiv:1911.00284)
- Move galaxies back to initial positions and infer the Gaussian density field at Lagrangian frame $\delta(q)$ with Hamiltonian Monte-Carlo (HMC)
- Then use nested Gibbs sampling Peculiar velocities, Displacements, Response function of the survey **Bias parameters**



COSMIC BIRTH

- **R** is the survey response operator $\delta_{obs} = \mathbf{R} \delta$
- $B(\delta)$ is the bias function, connecting number of galaxies to DM per cell $i \langle \rho_{Gal} \rangle_i = \overline{NR}_{ii}B(\delta_i)$: a nonlinear, nonlocal and stochastic function
- Real and redshift-space connected via peculiar velocity: $s = r + \frac{v_r}{H(a)a}$ $v_r = (v \cdot r)e_r$
- $\psi(q)$: displacement field using 2LPT



DENSITY SAMPLING

 $\delta(q) \curvearrowleft \mathscr{P}(\delta(q) | q, B(q), \mathbf{R})$

• Step II: Use the density field to infer Lagrangian real-space positions:

Step I: Assume tracers are in Lagrangian space q and sample density with HMC:

 $q \curvearrowleft \mathcal{P}(q \mid \delta(q), s, \psi)$



DENSITY SAMPLING

• Use Bayesian approach to define posterior of parameter Θ given the data d: $\mathscr{P}(\Theta | d) \propto \pi(\Theta) \times \mathscr{L}(d | \Theta)$, where data d is the galaxy counts per cell and parameters Θ are density values

$$\pi(\boldsymbol{\delta}_{\mathrm{L}}) = \frac{1}{\sqrt{(2\pi)^{N_c} \det(\mathbf{C}_{\mathrm{L}})}} \exp\left(-\frac{1}{2}\boldsymbol{\delta}_{\mathrm{L}}^{\mathrm{T}}\mathbf{C}_{\mathrm{L}}^{-1}\boldsymbol{\delta}_{\mathrm{L}}\right) \quad \boldsymbol{\delta}_{\mathrm{L}} = \log(1+\boldsymbol{\delta}) - \boldsymbol{\mu},$$

$$\mathscr{L}(N_{\rm G}|\lambda) = \prod_{i} \frac{\lambda_i^{N_{\rm Gi}} e^{-\lambda_i}}{N_{\rm Gi}!} \text{ in each cell } i$$



HAMILTONIAN MONTE CARLO

- Canonical posterior probability defined
- Variable of interest q in potential: $-\ln \mathcal{P}(q) = \mathcal{U}(q)$

• We use Hamilton dynamics for our probabilistic system $\mathcal{H}(q,p) = \mathcal{U}(q) + \mathcal{K}(p)$

d as:
$$\mathcal{P}(\boldsymbol{q},\boldsymbol{p}) = \frac{1}{Z} e^{-\mathcal{H}(\boldsymbol{q},\boldsymbol{p})}$$

• Kinetic term artificial to calculate Hamiltonian EoM: $\mathcal{P}(p) \propto e^{-\mathcal{X}} = e^{-\frac{1}{2}p^{T}M^{-1}p}$

• Link potential term to Bayesian posterior $-\ln \mathcal{P}(\delta_L | N_G) \propto -\ln \pi(\delta_I) - \ln \mathcal{L}(N_G | \delta_I)$



HAMILTON EQUATIONS OF MOTION

• Evolve HMC system according to Hamiltonian mechanics:

$$\frac{\mathrm{d}\boldsymbol{q}}{\mathrm{d}t} = \frac{\partial \mathcal{H}(\boldsymbol{q},\boldsymbol{p})}{\partial \boldsymbol{p}} = \mathbf{M}^{-1}\boldsymbol{p} \qquad \frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} = -\frac{\partial \mathcal{H}(\boldsymbol{q},\boldsymbol{p})}{\partial \boldsymbol{q}} = -\frac{\partial \mathcal{U}(\boldsymbol{q})}{\partial \boldsymbol{q}}$$

$$p\left(t+\frac{\epsilon}{2}\right) = p(t) - \frac{\epsilon}{2} \frac{\partial \mathcal{U}}{\partial q}(q(t)),$$
$$q\left(t+\epsilon\right) = q(t) + \epsilon \mathbf{M}^{-1} p\left(t+\frac{\epsilon}{2}\right),$$
$$p\left(t+\epsilon\right) = p\left(t+\frac{\epsilon}{2}\right) - \frac{\epsilon}{2} \frac{\partial \mathcal{U}}{\partial q}(q\left(t+\epsilon\right))$$

• For a pseudo time step $\Delta t = \epsilon$ we use 2nd order: $\mathcal{T}_2(\epsilon) = \mathcal{T}_p(\epsilon/2)\mathcal{T}_q(\epsilon)\mathcal{T}_p(\epsilon/2)$



HAMILTON EQUATIONS OF MOTION

Evolve HMC system according to Hamiltonian mechanics:

d q	$\partial \mathcal{H}(\boldsymbol{q},\boldsymbol{p}) = \mathbf{M}^{-1}\boldsymbol{p}$	$-1_{\mathbf{n}} \frac{\mathrm{d}\mathbf{p}}{-1_{\mathbf{n}}}$	дЖ
dt	др — IVI	P dt	

• Second Order: $\mathcal{T}_2(\epsilon) = \mathcal{T}_p(\epsilon/2)\mathcal{T}_q(\epsilon)\mathcal{T}_p(\epsilon/2)$

- $\mathcal{T}_{n+2}((2i-s)\epsilon) = \mathcal{T}_n^i(\epsilon)\mathcal{T}_n(-s\epsilon)\mathcal{T}_n^i(\epsilon), \text{ with:}$ $\Delta \tau_{4th} = (2i - s(n = 2)) e^{\text{eff}} = (2i - (2i)^{1/(3)}) e^{\text{eff}}$
- *i* is a free parameter of the scheme, we chose i = 4

$$\frac{\partial \mathcal{U}(q)}{\partial q} = \frac{\partial \mathcal{U}(q)}{\partial q}$$

Higher even order achieved by recursive application of second order leap-frog:



The dimensionality of the parameter space is in principle every single grid cell in the observed volume!



https://theclevermachine.wordpress.com/



PART II: CONSTRAINED SIMULATIONS

Ata et al 2022, Nature Astronomy, arXiv:2206.01115

- Environment of ~10 Mpc scales is decisive for the fate of a protocluster
- Previous works analysed singular protoclusters with simple methods (e.g. looking for analogous overdensities in N-body sims, simple analytic spherical overdensity estimate)
 - At the right time,
 - At the right position,

• Forms the right densities

Constrained Simulations





- COSTCO is a suite of 50 cosmological simulations run from HMC realisations of the COSMOS initial conditions $2 \le z \le 2.5$
- Cubic volume of 512 Mpc/h side length and 2 Mpc/h resolution $-> M_{\rm res} \sim 7 \times 10^{11} M_{\odot}/h$
- Identify massive halos at the z = 0 snapshot and trace back the member DM particles of each halo, defining the protocluster
- Match simulations to observations in position and mass

WELCOME TO COSTCO

(CONSTRAINED SIMULATIONS OF THE COSMOS FIELD)



CONSTRAINED SIMULATIONS OF COSMOS FIELD

- ~50000 MCMC samples of z=100 initial conditions produced by COSMIC BIRTH
- 50 random selected (thinning, autocorrelation length...) samples for simulations
- 256³ particles in a box with 512 Mpc/h side length (~7E11 Msun/h resolution)
- Simulations run from z=100 to z=0
- We write snapshots at z=2.5-2.0 in z = 2 2.5 $\Delta z = 0.1$ and z = 0
- Consistently used Planck 2018 cosmology from Initial Conditions to final analysis







COSTCO TIME EVOLUTION

Observed redshift distance z^{obs} 2.2 2.3

Observed redshift distance z^{obs} 2.2 2.3

2.4

400

2.4

2.5

2.5

200 300Line of Sight distance $[h^{-1} \text{Mpc}]$



$\begin{array}{c} \textbf{COSTCO TIME EVOLUTION} \\ \textbf{Observed redshift distance } z^{obs} \\ \textbf{2.1} \\ \textbf{2.2} \\ \textbf{2.3} \\$



Line of Sight distance $[h^{-1}Mpc]$





MATCH KNOWN PROTOCLUSTERS IN COSTCO

- 1. Identify massive halos at the z = 0 snapshot with $M_{\rm vir} \ge 2 \times 10^{14} h^{-1} M_{\odot}$
- of their Lagrangian region
- 3. Search in a radius of $r \leq 15 h^{-1}$ Mpc for reported protoclusters (e.g. Chiang+2017)
- 4. Average the findings over 50 realisations

2. Trace the member particles back to z = 2.3 and compute center of mass position



MATCH KNOWN PROTOCLUSTERS IN COSTCO



Line of Sight distance $[h^{-1} Mpc]$

Observed redshift distance z^{obs} 2.2 2.3 2.4 2.5 300 500 400





CLUSTER-PROTOCLUSTER

Center of Mass z = 2.3Halo position z = 0 $M_{\rm vir}(z=0) = 4.2 \times 10^{14} \, h^{-1} \, M_{\odot}$ 265--097 -1 Mpc] distance [h]255-Transverse 250-245-300.0 302.5 305.0 307.5 310.0 297.5 Line of Sight distance $[h^{-1}Mpc]$



Predicted Future Fate of COSMOS Galaxy Protoclusters over 11 Gyrs with Constrained Simulations

https://www.youtube.com/watch?v=IIqCZUb-OqQ

Metin Ata et al. (2022)



150.0 150.2 150.4 150.6 RA



- ZFIRE and Hyperion appear in all realisations
 - will likely become a very massive $M \sim 2.5 \times 10^{15} h^{-1} M_{\odot}$ filament with an spatial extent of ~ $65 h^{-1}$ Mpc
- Confirm CC2.2 (Darvish+2020)
- Disfavor CCPC-z22-006 (Franck+2016)
- Inconclusive on G237 (Polletta+2021)
- 5 new protoclusters discovered in COSMOS!

RESULTS

• While ZFIRE is an isolated structure of $M \sim 1.2 \times 10^{15} h^{-1} M_{\odot}$, Hyperion

Name [Ref.]	R.A. [deg]	Dec [deg]	$z^{ m obs}$	Final Mass $[h^{-1}]$
ZFOURGE/ZFIRE [9, 10]	150.094	2.251	2.095	$(1.2 \pm 0.3) \times 10^{15}$
G237* [19]	150.507	2.312	2.16	
CC2.2* [18]	150.197	2.003	2.232	$(4.2 \pm 1.9) \times 10^{14}$
CCPC-z22-006 [11]	149.930	2.200	2.283	
	150.093	2.404	2.468)
	149.976	2.112	2.426	
	149.999	2.253	2.444	
Hyperion [12–17]	150.255	2.342	2.469	$(2.5 \pm 0.5) \times 10$
	150.229	2.338	2.507	
	150.331	2.242	2.492	
	149.958	2.218	2.423	J
COSTCO J100026.4+020940	150.110	2.161	2.298	$(4.6 \pm 2.2) \times 10^{14}$
COSTCO J095924.0+021435	149.871	2.229	2.047	$(6.1 \pm 2.5) \times 10^{14}$
COSTCO J100031.0+021630	150.129	2.275	2.160	$(5.3 \pm 2.6) \times 10^{14}$
COSTCO J095849.4+020126	149.706	2.024	2.391	$(6.6 \pm 2.3) \times 10^{14}$
COSTCO J095945.1 + 020528	149.938	2.091	2.283	$(4.3 \pm 2.4) \times 10^{14}$



MIND THE ORPHANS

- Stack all 50 COSTCO N-body runs into one volume: The COSTCO Multiverse •
- Identify protoclusters that are forming in significantly many realisations (28 of 50) •
- **DBSCAN** multiverse clustering analysis •





MIND THE ORPHANS

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MATCHING THE ORPHANS





COSTCO HALO MASS FUNCTION

- Are there too many massive protocluster progenitors in COSMOS at 2<z<2.5?
- size, resolution, ...)
- Number of ~10¹⁵ h⁻¹ M_{\odot} halos in COSTCO is consistent with global Λ CDM



Compare the COSTCO halo mass function with a set of random simulation with same setup (box



- Constrained simulations now allow direct modeling of galaxy protoclusters:
 - "Fast forward" to z=0 to measure their final cluster masses
 - Hyperion will collapse into a giant supercluster filament (~100 cMpc long)
 - 5 new protoclusters discovered in existing data
- Follow-up projects:
 - Galaxy properties as a function of matter density field (Rieko Momose)
 - Quasar Lyman-alpha forest absorption as a function of matter density field (Ilya Khrykin)
 - Comparison with CLAMATO IGM Tomography (Chenze Dong)

SUMMARY

Application of density reconstruction and constrained simulations to COSMOS spectroscopic data at 2.0<z<2.5

