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Full Text

Preamble

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Mock X-Ray Observations of Hot Gas with L-Galaxies Semi-analytic Models of Galaxy Formation

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Abstract

We create mock X-ray observations of hot gas in galaxy clusters with a new extension of the L-Galaxies semi-analytic model of galaxy formation, which includes the radial distribution of hot gas in each halo. Based on the model outputs, we first build mock light cones, then generate mock spectra with the SOXS package and derive mock images in the light cones. Using the mock data, we simulate X-ray spectra for the ROSAT all-sky survey and compare them with observational results. Then, we consider the design parameters of the HUBS mission and simulate observations of halo hot gas for HUBS as an important application of our mock work. We find: (1) our mock data match observations by current X-ray telescopes; (2) the survey of hot baryons in resolved clusters by HUBS is effective below redshift 0.5, and observations of emission lines in point-like sources at $z > 0.5$ help us understand hot baryons in the early universe; (3) by taking advantage of the large simulation box and flexibility in semi-analytic models, our mock X-ray observations provide opportunities to select targets and optimize observation strategies for forthcoming X-ray facilities.

Key words: X-rays: galaxies: clusters -galaxies: clusters: intracluster medium -galaxies: groups: general -galaxies: halos -(galaxies:) intergalactic medium

1. Introduction

According to ΛCDM cosmological models and results from Planck, baryonic matter contributes about 4.9% of the total mass in the universe (Planck Collaboration et al. 2020), and consists of cold baryons locked in galaxies (stars, interstellar medium (ISM), black holes, etc.; Kravtsov & Borgani 2012) and hot baryons in diffuse and ionized phases in circumgalactic medium (CGM) and intracluster medium (ICM). According to observations (Shull et al. 2012) and simulation work (e.g., Cen & Ostriker 2006), cold baryons contribute less than 15% of the baryon budget and hot gas dominates the baryon content in the low-redshift universe.

X-rays emitted by hot baryons can test cosmological models and provide important information on the baryon and energy cycles of galaxies and clusters, as well as trace how dark matter structures assembled on large scales. In the past two decades, surveys by the X-ray telescopes XMM-Newton and Chandra have detected X-ray emission from hot haloes around galaxies (e.g., Li & Wang 2013; Li et al. 2017; Babyk et al. 2018). ROSAT completed the first X-ray imaging all-sky survey in the soft X-ray band (RASS, Voges et al. 1999) and provided catalogs for thousands of galaxy clusters (e.g., Piffaretti et al. 2011; Finoguenov et al. 2020). The new X-ray telescope eROSITA completed the Final Equatorial-Depth Survey (eFEDS) by the end of 2019 (Brunner et al. 2022), which is a verification of the eROSITA all-sky survey (eRASS). The catalog from eFEDS, which includes 542 candidates of galaxy clusters detected as extended X-ray sources in the 140 deg^2 sky area, helps in the study of CGM and ICM properties (Bahar et al. 2022; Liu et al. 2022).

A number of large-scale X-ray surveys are proposed to improve our understanding of hot baryons in the foreseeable future. eROSITA will complete eight all-sky surveys in the soft X-ray band by the end of 2023 (eRASS:8), yielding a sample of over 10^5 galaxy clusters (Merloni et al. 2012; Predehl et al. 2021). The X-ray survey by Athena Phase B will extend the study of hot baryon distributions in ICM by mapping the properties of low-mass groups up to z 2 (Ettori et al. 2013; Kaastra et al. 2013). The Wide Field Imager (WFI) survey, during its first four years of operation, is predicted to detect over 10,000 groups and clusters with $z > 0.5$, including 20 groups with a mass of $M_{500} > 5 \times 10^{13}$ M at around z 2 (Zhang et al. 2020). The Chinese HUBS mission (Cui et al. 2020) intends to conduct an all-sky survey of hot baryons in warm-hot ionized medium and CGM with its large field of view and high spectral resolution (see Table 2 in Section 3.2 of this paper).

On the other hand, recent cosmological hydrodynamic simulations such as EAGLE (Crain et al. 2015; Schaye et al. 2015) and Illustris-TNG (Nelson et al. 2018; Springel et al. 2018) predict hot haloes around groups and clusters. Many papers study X-ray emission from ICM and CGM using simulation results (e.g., Stevens et al. 2017; Kovacs et al. 2019; Martizzi et al. 2019; Truong et al. 2021), and some works further make mock X-ray observations based on plans of X-ray surveys. For example, Oppenheimer et al. (2020) makes predictions of resolved X-ray images for eROSITA with EAGLE and Illustris-TNG. Wijers & Schaye (2022) discusses prospects for detection of X-ray emission lines for Athena X-IFU and Lynx Main Array (Gaskin et al. 2019) using EAGLE. Zhang et al. (2022) creates mock observations for HUBS with Illustris-TNG and assesses scientific capabilities for detecting extended X-ray emission from hot gas. Vijayan et al. (2022) generates X-ray emission of ISM and CGM from MACER code (Yuan et al. 2018), and simulates HUBS observations of elliptical galaxies in four sets of simulations.

The outputs of semi-analytic models of galaxy formation (hereafter SAMs) offer another choice to build mock observations, such as the mock observatory by Overzier et al. (2013), mock cones for SKA H I Surveys by Obreschkow & Meyer (2014), and mock galaxy catalogs in multiple bands by Merson et al. (2013). Due to the low cost of running SAMs, the main advantage of their outputs is the large size of the simulation box (e.g., the box size of L-Galaxies SAMs is 500 Mpc h^{-1} based on Millennium Simulation, Henriques et al. 2015). The large simulation box helps in constructing mock observations of a very large sky area without the effect of cosmic variance even at high redshift; the 500 Mpc h^{-1} box corresponds to a sky area of over 50 deg^2 at z 2.0. The mock catalog based on Millennium Simulation (Springel et al. 2005) can also contain hot gas in very massive haloes ($M_{200} > 10^{15}$ M). On the other hand, the flexibility of SAMs makes it possible to generate multiple mock observations based on outputs with different model parameters and prescriptions, which enables investigation of the effect of physical processes and model parameters on observational results (Somerville & Davé 2015).

In our recent work (Zhong et al. 2023, hereafter Paper I), we develop a new extension of L-Galaxies 2015 SAMs (Henriques et al. 2015) to study the ionized hot gas in haloes. In contrast to most previous SAMs work (e.g., L-Galaxies 2020 by Henriques et al. 2020; DARK SAGE by Stevens et al. 2016; Shark by Lagos et al. 2018), which mainly focuses on stellar and cold gas components in galaxy disks and ISM, Paper I concentrates on properties and spatial distribution of hot baryon components, as well as corresponding X-ray emission from hot gaseous haloes. Our model results successfully reproduce various X-ray observations, such as radial profiles of hot gas temperature, scaling relations of X-ray luminosity, and baryon fraction in haloes with different masses.

In this paper, we create mock X-ray observations of halo hot gas based on the outputs of the SAMs in Paper I. First, we build mock light cones using the resulting spatial information, then generate mock spectra and images in the soft X-ray band based on physical properties. We consider instrument parameters of X-ray facilities to mimic observations, particularly for the HUBS mission. The mock results presented in this paper will aid in optimization of target selection and observation strategies for future X-ray surveys of hot gas, and they can also be compared to mock results from other simulations.

This paper is organized as follows. In Section 2, we describe the methodology used to create mock X-ray observations for hot gas in haloes, including steps to build mock light cones and procedures to generate mock spectra and images. We also show examples of mock images and spectra of galaxy clusters. In Section 3, we consider instrument parameters of X-ray telescopes and simulate observations based on mock data. We simulate mock spectra for ROSAT as a benchmark and then focus on mock observations for the HUBS mission. In Section 4, we summarize this paper and look ahead to future work.

2. Methods

In this section, we describe how to create mock X-ray observations of hot gas using model outputs from L-Galaxies SAMs. We first describe steps to build mock light cones, then procedures to generate mock spectra and images of galaxy clusters in the light cones. It should be noted that we do not distinguish between definitions of galaxy “group” and “cluster” in the following sections; both denote a collection of galaxies embedded in the same dark matter halo, and we use the term “cluster” for simplicity.

2.1. Simulation and Model Samples

The mock observations in this paper are based on outputs from the models in Paper I, in which we developed a new branch of the L-Galaxies 2015 (Henriques et al. 2015) SAMs to describe the radial distribution of hot ionized gas in ICM and CGM. In Paper I, we use a physical model that accounts for local instabilities and thermal equilibrium processes for hot gas in haloes to replace the isothermal sphere in previous models. The model outputs include one-dimensional radial profiles of hot gas density, gas temperature, and bolometric X-ray luminosity profiles around each dark matter halo. The model results successfully reproduce X-ray observations, such as radial profiles of hot gas density (e.g., the electron density profile from REXCESS by Croston et al. 2008 and the gas temperature profile from XMM-Newton and Chandra by Bartalucci et al. 2017), scaling relations of X-ray luminosity and temperature (Goulding et al. 2016 and Babyk et al. 2018 from Chandra; Mulchaey et al. 2003 and Anderson et al. 2015 from ROSAT; Li et al. 2016 from XMM-Newton), and baryon fraction in different haloes (Gonzalez et al. 2013 from XMM-Newton; Vikhlinin et al. 2006 and Sun et al. 2009 from Chandra).

In this paper, the SAMs results used to build mock observations are based on dark matter haloes from the Millennium Simulation (hereafter MS, Springel et al. 2005), rescaled to Planck cosmological parameters ($\Omega_\Lambda = 0.685$, $\Omega_m = 0.315$, $\Omega_{baryon} = 0.0487$, $\sigma_8 = 0.829$, and h = 0.673, Planck Collaboration et al. 2020). The comoving box size is about 480 Mpc h^{-1} or 713 Mpc on a side, which is several times larger than recent cosmological hydrodynamic simulations such as EAGLE (in a box of 100 Mpc) and Illustris-TNG (in a box of 100 Mpc or 300 Mpc). The minimum halo mass is about 2.9×10^{10} M , which is the mass of 20 simulated particles. The resolution of MS is high enough to mimic observations of the hot gas component in most galaxy clusters, and emission from hot gas in haloes below this resolution is usually undetectable in the soft X-ray band. Based on model results in Paper I, the gas temperature in haloes smaller than 10^{11} M tends to be lower than 0.1 keV.

The SAMs results are saved as halo and galaxy catalogs in a series of discrete snapshots, each corresponding to a certain redshift z. Based on halo merger trees of MS rescaled to Planck cosmological parameters, the model outputs include 59 snapshots from redshift z 56 to z = 0. The catalogs include details of spatial positions and physical properties of each halo and galaxy.

Based on model prescriptions in Paper I, properties of hot gas in each halo, including gas density _{hot} and bolometric X-ray emission profiles L_X, are stored in the form of "radial profiles," corresponding to values in a set of spherically symmetric shells with certain radii around the halo center. To mimic real observations, luminosity profiles in concentric 3D shells are projected to surface brightness in 2D rings:

$$I_{X,j} = \frac{\sum_i L_{X,i} f_{V,ij}}{A_j}$$

where L__X,i (unit: erg s^{-1}) is the bolometric X-ray luminosity in shell i, and I__X,j (unit: erg s^{-1} kpc^{-2}) is the projected X-ray surface luminosity in ring j. f__V,ij represents the volume fraction of shell i projected in ring j, and A__j is the projected area of ring j. Detailed formulae and discussions on the projection can be found in papers such as McLaughlin (1999) and Ettori (2002).

In Figure 1 [Figure 1: see original paper], we show an illustration of the hot gas component in model outputs at z = 0, one of the snapshots used to construct light cones and mock observations. The illustration is in a subbox of the MS volume with about 60 Mpc h^{-1} on a side. In this figure, each dot represents one hot gaseous halo, and the size and color of each dot represent the virial radius R_{200} and bolometric X-ray luminosity of each halo.

In the framework of SAMs, we have "halo hot gas" in model results and do not distinguish between ionized hot gas in ICM or CGM, concentrating only on X-ray emission from hot gas components inside the virial radius of each halo. We should also mention that SAMs do not consider details of nonspherical structures such as filaments, knots, and cosmic webs. The baryons in these structures are thought to reside in the hot gas halo or the ejecta reservoir outside the halo depending on whether they are bounded within the halo potential.

2.2. Light Cones

Model results for haloes and galaxies are in cubic simulation boxes at a finite number of redshifts. To mimic real observations, we convert cubic boxes into virtual sky information (3D positions and 3D velocities). We follow methods (MoMaF) developed by Blaizot et al. (2005) and Kitzbichler & White (2007) to create mock catalogs and light cones based on SAMs outputs; details can be found in the original papers and subsequent works (e.g., Obreschkow et al. 2009; Zoldan et al. 2017). Here we briefly describe the steps:

(i) We position the observer at coordinate origin (0, 0, 0) and randomly replicate simulation boxes in a 3D grid. First, we calculate comoving distance from a box center to the observer and get the corresponding redshift, then we stack the box with the closest redshift. Due to the relatively large simulation box size (L__{box} 710 Mpc for MS), it is not necessary to use model outputs in each snapshot at low redshift. We truncate the 3D grid at z 2, which includes $8^3 = 512$ MS boxes. According to forthcoming plans for X-ray telescopes, z 2 corresponds to the redshift limit of massive cluster surveys by eRASS (Merloni et al. 2012), and also the redshift limit of warm-hot baryon and cluster observations by Athena (Nandra et al. 2013).

In our current work, we simply splice boxes at different snapshots together to get a continuous cubic 3D grid and light cones, similar to work by Zoldan et al. (2017) and Comparat et al. (2020). However, this simplified method may lead to discontinuities in light cones because of discrete redshift bins in model outputs. In some mock observation work, authors interpolate positions and velocities of haloes and galaxies between snapshots (e.g., Merson et al. 2013; Smith et al. 2022), and even intrinsic properties (stellar mass, gas mass, star formation rate, etc.) of each galaxy (Barrera et al. 2022). According to results and discussions in Merson et al. (2013) and Smith et al. (2022), interpolation mainly affects results of galaxy clustering and color assignment. In this paper, our mock observations mainly focus on X-ray images and spectra of hot gaseous haloes, and clustering and distribution on large scales do not affect our mock results. On the other hand, we adopt an energy band with continuous redshift in dealing with mock images and spectra (see details in Sections 2.3 and 2.4) at high redshift, which avoids producing discrete color distributions in results.

(ii) To suppress spurious radial features caused by repeated boxes, we assign "random tiling" on the 3D grid, which includes random operations of shift, rotation, and inversion on 3D coordinates and velocities.

(iii) In the stacked 3D grid, we calculate comoving coordinates (r__x, r__y, r__z) of each object relative to the observer and convert them to spherical coordinates (α, δ, z). The R.A. α and decl. δ are calculated as:

$$\alpha = \arctan\left(\frac{r_y}{r_x}\right), \quad \delta = \arctan\left(\frac{r_z}{\sqrt{r_x^2 + r_y^2}}\right)$$

Since mock samples should have continuous redshift distribution instead of discrete model outputs, we calculate redshift z of each source from its comoving distance d:

$$d = \int_0^z \frac{c\,dz'}{H_0\sqrt{\Omega_m(1+z')^3 + \Omega_\Lambda}}$$

where Ω__Λ and Ω__m are cosmological parameters. The apparent redshift z__v with Doppler shift is then calculated as:

$$1 + z_v = (1 + z_{\cos})(1 + v_r/c)$$

where v__r is the peculiar velocity projected along the line of sight, and z__{cos} is the cosmological redshift from Equation (3).

(iv) Based on model outputs in spherical coordinates mentioned above, we create light cones to mimic real observations. Considering the field of view of HUBS (1 deg^2) and eROSITA (1.03° × 1.03°), we choose 1° × 1°

as the angular size of each light cone. Mock data are saved according to light cones. We generate two sets: one deep light cone and several shallow ones. The deep light cone is generated in a random direction up to z 2. The 10 shallow light cones are generated up to z 0.2, and the center of each is a nearby cluster. Furthermore, it is quite easy to generate more light cones for further statistical analysis.

Based on model results in Paper I, we focus on mock data of haloes with $M_{200} > 10^{12}$ M , since hot gas temperature in haloes around 10^{12} M is just above 0.1 keV, and emission from lower-mass haloes is nearly invisible in the soft X-ray band. The deep light cone up to z 2 contains approximately 24,000 haloes above 10^{12} M , and shallow light cones up to z 0.2 contain around 73 haloes above 10^{12} M on average.

In Figure 2 [Figure 2: see original paper], we show the redshift distribution per redshift bin ($\Delta z = 0.2$) per square degree of haloes with $M_{200} > 10^{12}$ M , averaged throughout the entire mock sky up to $z = 2$. We can see that the number of haloes per square degree peaks at z 1 and changes little at higher redshift.

2.3. Mock Spectra

To generate mock spectra of X-ray emission from halo hot gas, we use the package "Simulated Observations of X-ray Sources" (SOXS), whose details can be found on the SOXS webpage (https://hea-www.cfa.harvard.edu/soxs). In the SOXS package, we apply the APEC spectrum generator based on hot plasmas in collisional ionization equilibrium (Foster et al. 2012) and also consider Galactic foreground absorption in the spectrum.

In each mock light cone, we generate a wide-band spectrum for hot gas in each halo and also narrow-band spectra around certain emission lines (e.g., the O VII and Fe XVII lines). To generate these spectra, the following three properties from L-Galaxies model outputs are used as input parameters for SOXS:

- F__X,bol: bolometric X-ray flux of hot gas in a halo
- T__X: luminosity-weighted mean gas temperature of a halo
- Z__{gas}: mean hot gas metallicity of a halo

The gas metallicity Z__{gas} is defined as the metallicity in hot gas relative to the solar value:

$$Z_{\rm gas} = \frac{M_{Z,\rm hot}}{M_{\rm hot} Z_{\odot}}$$

where M__Z,hot is the mass of metal elements in the hot phase and M__{hot} is the mass of the hot gaseous halo. The solar metallicity Z__ is set to 0.02. We note that the SAMs adopted in this paper do not contain abundances of different elements but only one value of total metallicity in hot gas.

For haloes at high redshift, we make redshift corrections on mock spectra. Considering f_o and f_e (unit: counts s^{-1} keV^{-1} cm^{-2}) as spectra in observed and emitted frames, the relation between f_o and f_e can be written as:

$$f_o(\nu_o) = \frac{f_e(\nu_e)}{1+z}$$

where _o is the frequency in the observed frame. Then we get spectra in the band of the observed frame.

2.4. Mock Images

To mimic observations, generating mock images is another important task. Using the projected surface luminosity profile in Equation (1) and mock spectra from Section 2.3, we obtain mock X-ray images for each halo in the light cone.

For a nearby halo with comoving distance d_c, the emissivity S_ (unit: erg s^{-1} cm^{-2} $arcmin^{-2}$) in a given band   is:

$$S_\nu = \frac{E_\nu}{E_{\rm bol}} \frac{I_{X,i}}{A_i}$$

where E_ and E_{bol} (unit: erg s^{-1}) represent X-ray emission energy in given band   and bolometric energy from the mock spectrum respectively. I_X,i (unit: erg s^{-1} kpc^{-2}) from Equation (1) is the projected surface brightness of bolometric luminosity in ring i of the model halo, and A_i is the projected area of ring i.

For high-redshift haloes in the deep light cone, redshift correction is made in calculation of surface brightness. Similar to K-correction in magnitude (e.g., Hogg et al. 2002), the emissivity S_ o in a given band _o is:

$$S_{\nu_o} = \frac{E_{\nu_e}}{E_{\rm bol}} \frac{I_{X,i}}{A_i} (1+z)^{-4}$$

where subscripts e and o represent quantities in emitted and observed frames respectively, and the term $(1+z)^{-4}$ represents redshift correction of surface brightness. On the other hand, due to cosmological redshift of the emitter, the observer can detect X-ray emission from gas with higher temperature in high-redshift clusters.

With the distribution of S_ , we get the emissivity image for a cluster (see examples in Section 2.5). Considering instrument parameters of a specific X-ray telescope, such as ancillary response file (ARF), redistribution matrix file (RMF), point-spread function (PSF), and exposure time, we can convert emissivity to photon-count density (unit: counts $arcmin^{-2}$) and generate mock images for each cluster in the light cones (details can be found in following sections).

In summary, we adopt model outputs from SAMs in Paper I to create mock X-ray observations of hot gaseous haloes. In Figure 3 [Figure 3: see original paper], we show a flowchart describing steps and procedures in this section. Here we briefly summarize:

1. We adopt L-Galaxies model outputs running on MS halo merger trees, stored in cubic boxes in discrete redshift bins.
2. Based on spatial information (3D positions and velocities) of each halo, we stack simulation boxes in a 3D grid and assign "random tiling" to suppress spurious radial features. Then we convert Cartesian coordinates of each halo to spherical coordinates with respect to the observer.
3. We generate light cones up to different redshifts with angular size 1° × 1°.
4. Using physical properties (X-ray flux, gas temperature, and gas metallicity) from model outputs, we generate mock X-ray spectra of hot gas in each halo with SOXS packages.
5. We project X-ray luminosity profiles in 3D shells to 2D surface brightness I_X,i and derive X-ray emissivity images with mock spectra. For haloes at high redshift, corrections are made on mock spectra and images.
6. Considering instrument parameters, we simulate observations for X-ray telescopes (see following sections).

2.5. Examples of Mock Images and Spectra for Clusters

In this subsection, we show mock images and spectra of hot gas in clusters at different redshifts. Considering methods of removing contamination and identifying cluster members by cross-matching X-ray sources with samples from multiple wavelengths (e.g., Salvato et al. 2022), mock images and spectra shown hereafter are based on clusters in our mock data. We identify members of a mock cluster through the halo merger tree in MS; all central galaxies (Types 0 and 1) and satellite galaxies (Type 2) in subhaloes (substructure within the larger virialised halo) of a main friends-of-friends (FoF) halo belong to one cluster. The boundary of each emission profile is located at the virial radius R_{200} of each subhalo, and satellites beyond the outer boundary of the central galaxy belong to another subhalo.

The current version of L-Galaxies SAMs includes hot baryons beyond the halo potential of a cluster (the ejected reservoir). However, the model does not consider structure and distribution of the unbounded reservoir, so all mock X-ray emission is from gas inside the halo boundary. Although baryons outside the halo potential are significant, they are very difficult to probe (Walker et al. 2019; Nicastro et al. 2022), and future model work on spatial distribution of unbounded gas in SAMs should be meaningful (Ayromlou et al. 2022).

To mimic observation of hot gas in nearby and high-redshift clusters, we show examples of mock spectra and emissivity images from three model clusters at different redshifts in Figure 4 [Figure 4: see original paper]. In the left column, we select a cluster with halo mass similar to the Milky Way (M_{200} 4×10^{12}

M at z 0.03) from one of the shallow light cones to mimic observation of a nearby cluster. For higher redshift results, the two mock clusters are from the deep light cone. The middle column shows a cluster with M_{200} 4×10^{14} M at z = 0.51, representing a cluster close to the redshift limit of the HUBS mission for observation of extended sources (see Section 3.2 for details). In the right column, we select a cluster with M_{200} 1.6×10^{14} M at z = 2.07, around the redshift limit of cluster detection for eROSITA and Athena. To show satellite structures more clearly, we also select a cluster with M_{200} 5×10^{14} M at z 0.047 and show its emissivity image in Figure 5 [Figure 5: see original paper], representing a nearby rich cluster with many substructures and satellite galaxies around the central galaxy. In each panel of emissivity images in Figures 4 and 5, the largest source represents X-ray emission from hot gas around the central galaxy and other sources are from satellite galaxies.

The X-ray emissivity images of these clusters are in the 0.1–2 keV band, and the field of view (hereafter FoV) of images in Figure 4 is 0.5° × 0.5°, while that in Figure 5 is 1° × 1°. We can see that all X-ray sources are spherical because the L-Galaxies model assumes a spherically symmetric profile for each hot gaseous halo. The outer boundary of each emission profile is located at the virial radius R_{200} of each subhalo.

The emissivity images of nearby clusters in Figures 4 and 5 indicate that many X-ray facilities are capable of detecting structures like spatial distribution of satellites and spatially resolved spectra of entire clusters. For the cluster at z 2 in the right column of Figure 4, the angular size is around 2 , which is around the limit of HUBS (1.0 arcmin angular resolution, Cui et al. 2020), while eROSITA (15 arcsec angular resolution, Merloni et al. 2012) and Athena (5 arcsec angular resolution, Kaastra et al. 2013) have the ability to resolve hot gas in central and large satellite galaxies.

The bottom three panels of Figure 4 present mock X-ray spectra of clusters shown in the top panels. In each panel, we stack all spectra from central and satellite galaxies together to get a single spectrum for each cluster. In the left panel for the nearby cluster, we can see bumps in the 0.5–1.0 keV band, which are emission lines of elements O, Fe, Ne, Mg, etc.; we will show details in narrow-band spectra in Section 3.2. The relatively high gas temperature (mean T_{gas} 2.5 keV) in this massive halo leads to high ionization fraction for some elements and weak plasma emission lines. On the other hand, high-redshift clusters extend the spectrum of the emitted frame to bands of high-energy processes, such as active galactic nuclei (AGNs) and black hole accretion. The current L-Galaxies SAMs include prescriptions of gas accretion and AGN feedback processes by central black holes (radio-mode accretion), but X-ray emission from AGNs and black holes is not included.

Some works suggest that AGN feedback affects X-ray luminosity of haloes to some extent. Gaspari et al. (2014) shows that purely AGN feedback lowers luminosity and heats gas. Puchwein et al. (2008) finds that AGN feedback significantly reduces X-ray luminosities of poor clusters and groups. Thus, to get more accurate mock X-ray observations for high-redshift clusters, future work on prescriptions of X-ray emission from black hole accretion and AGN feedback in SAMs is important.

3. Mock Observations for X-ray Telescopes

In this section, we consider instrument parameters of real X-ray facilities and simulate observations of hot gas based on our mock data. As a benchmark, we first simulate X-ray spectra of the ROSAT all-sky survey and compare mock results with observations. Then we focus on mock observations for the future HUBS mission.

3.1. Mock Spectra of Clusters for the All-sky Survey

In this subsection, we simulate spectra of clusters in the first X-ray all-sky survey (RASS) by ROSAT (Voges et al. 1999) as an application of our mock spectra.

Following procedures in Dai et al. (2007), we select clusters from the mock sky up to z 0.2 and place them at a common distance of 100 Mpc to normalize apparent luminosity. In Dai et al. (2007), RASS clusters are divided into several groups according to optical richness, and the richness parameter N_{666}* has a fitting relation with bolometric X-ray luminosity L_X of a cluster. Similarly, our mock clusters are divided into four groups based on L_X, and parameters of each group are listed in Table 1 .

Since RASS images have already corrected exposure times for vignetting effects, we use the on-axis effective area A_{eff} from Table 5.3 in the ROSAT handbook to generate mock spectra comparable with RASS results. The power F( ) (unit: counts s^{-1} keV^{-1}) received by ROSAT at frequency is:

$$F(\nu) = f(\nu)A_{\text{eff}}(\nu)$$

where f( ) (unit: counts s^{-1} cm^{-2} keV^{-1}) is flux of a mock spectrum generated by the SOXS package. In addition, Galactic foreground absorption is considered when calculating f( ) in Equation (11), and column densities N_H of foreground absorption are listed in the last column of Table 1, same as values used in Dai et al. (2007).

Figure 6 [Figure 6: see original paper] shows X-ray spectra in the 0.1-2 keV band derived from mock clusters together with observational spectra from RASS by Dai et al. (2007). Samples are divided into four panels according to L_X and N_{666}* in Table 1. In each panel, the trough in the spectrum at around 0.5 keV is caused by drop in ROSAT sensitivity between 0.3 and 0.6 keV, and the drop at E 0.2 keV is caused by foreground absorption.

As shown in Figure 6, mock spectra can roughly match results from RASS in the 0.1-2 keV band, with the main difference in Group 4 (clusters with L_X > $10^{43\cdot5}$ erg s^{-1}). In these bright clusters, flux of the mock sample at E < 0.5

keV is slightly higher than that of RASS, meaning the model predicts lower gas temperature T_X than observations in massive haloes. For clusters in Group 4, the average gas temperature from RASS clusters is T_X = 3.5 keV, while T_X = 2.7 keV for the mock sample. According to scaling relations of hot gas in Paper I (detailed discussions on scaling relations can be found in Section 3.2 of that paper), the inconsistency in bright clusters is primarily caused by too steep a slope of the L_X-T_X relation in mock clusters. To fit the relation L_X,bol   T_X^4.5 for early-type galaxies in the range L_X 10^{38}-10^{43} erg s^{-1} from Chandra (Babyk et al. 2018), Paper I gives the model result L_X,bol   T_X^5.5, which is steeper than slopes of clusters in RASS (L_X,bol   T_X^3.0 ± 0.3, Dai et al. 2007) and eFEDS (L_X,bol   T_X^3.0, Bahar et al. 2022). On the other hand, according to discussion at the end of Section 2.5, AGN feedback suppresses X-ray luminosity to some extent. Since the current model does not contain X-ray emission from AGNs, this should be another cause of discrepancy in the L_X-T_X relation in massive clusters. Future work is necessary to improve model prescriptions in bright clusters with L_X $> 10^{43}$ erg s^{-1}.

3.2. Mock Observations for HUBS

HUBS (The Hot Universe Baryon Surveyor) is a mission scheduled to launch around 2030 in China. Thanks to its large 1 deg^2 FoV, HUBS is at least an order of magnitude more capable than small-FoV X-ray telescopes at detecting diffuse emission from hot gas thought to hide in CGM and IGM. According to observing strategy (Cui et al. 2020), HUBS plans to observe nearby galaxies and clusters with quite long exposure times (1 Ms), and target selection is very important for achieving science objectives. On the other hand, main advantages of SAMs are the large simulation box and flexibility to investigate effects of physical processes. In this section, we simulate images and spectral observations of HUBS using our mock data of hot gas based on SAMs. This is an important application of our mock work that may aid in optimizing future observations for the HUBS mission.

To simulate observations of the HUBS mission, we adopt key design parameters from Cui et al. (2020), shown in Table 2 . It should be noted that effective area A_{eff} in Table 2 is a function of energy from the ancillary response file (ARF) by Zhang et al. (2022), used to convolve with flux f( ) to get photon counts. In each light cone, we generate wide-band and narrow-band mock spectra for each cluster, where wide-band spectra are in the 0.1–2 keV band with regular energy resolution of 2 eV while narrow-band spectra are in bands around emission lines with resolution of 0.6 eV. Considering effective area, angular resolution, and exposure time of HUBS, we derive photon images in both wide and narrow bands using count emissivity maps and spectra of each cluster.

In generation of mock images and spectra, foreground and background are also included. According to results from XMM-Newton by Lumb et al. (2002), the cosmic unresolved X-ray background (hereafter XRB) emission is modeled with a power-law spectrum:

$$S_b(E) = 7.9 \times 10^{-9} \left(\frac{E}{1\,\mathrm{keV}}\right)^{-1.29} \mathrm{erg\ cm^{-2}s^{-1}keV^{-1}sr^{-1}}$$

Considering effective area A_{eff} of HUBS, the background count rate can be calculated as:

$$n_b = \int_{0.1}^{2.0} S_b(E) A_{\mathrm{eff}}(E)\, dE$$

where A_{eff} is a function of energy from the ARF by Zhang et al. (2022). Then we get the value of n_b in the 0.1-2.0 keV band: n_b = 0.02 counts arcmin^{-2} s^{-1}.

For the foreground, we assume a constant column density N_H = 2 × 10^{20} cm^{-2} (Willingale et al. 2013) for Galactic foreground absorption, which mainly affects the band below 0.3 keV.

In Paper I, our model results predict that haloes between 10^{12} and 10^{13} M tend to contain a large fraction of hot gas with temperature below 0.5 keV, which is hard for many X-ray facilities to detect (Paerels et al. 2008). Thus, we select a nearby cluster with M_{200} 5×10^{12} M at z 0.014 from one of the shallow light cones and show X-ray mock images in Figure 7 [Figure 7: see original paper]. This is a typical cluster in our mock sample, representing a Local Group-sized halo in the nearby universe, similar to a potential target of the HUBS mission (Cui et al. 2020).

The four panels of Figure 7 show the emissivity image, wide-band image, and narrow-band images around O VIII and Mg XI emission lines. Emissivity and wide-band images are in the 0.1-2 keV band, and wide-band and narrow-band images are calculated with an exposure time of 10^6 s. In addition to the cluster in the center of the light cone, images also include emission from other sources in the 1 deg^2 FoV. We note that all sources in mock images contain only X-ray photons from hot gas, and our current SAMs outputs do not include X-ray emission from other sources such as AGNs and X-ray binaries. To improve contrast, photons from the XRB are not shown in Figure 7. Considering the background count rate of HUBS, images in Figure 7 show that HUBS is capable of detecting X-ray emission from most hot gas inside the virial radius R_{200} of the nearby cluster with an exposure time of 10^6 s.

Figure 8 [Figure 8: see original paper] shows X-ray spectra of the cluster in the center of Figure 7. To mimic contamination sources in the spectra, we include contributions of all sources in the solid angle of R_{200} to the cluster center in the light cone, and superpose redshifted spectra from contamination sources onto the spectrum of the central cluster. The top panel shows the wide-band spectrum at 0.1-2 keV and bottom panels show zoomed-in narrow-band spectra around emission lines of C VI, O VII, O VIII, Fe XVII, Ne X, and Mg XI.

In each panel, the dashed curve shows the spectrum of the XRB, representing background noise. The drop at the left end of the wide-band spectrum is caused by Galactic foreground absorption and decrease in effective area below the 0.3 keV band.

Based on mock data, we can also predict the number of sources detectable by HUBS at different redshifts. We assume most baryons in a cluster can be detected if the signal-to-noise ratio (S/N) is greater than 10 inside radius R_{500} of the halo (R_{500} is the radius within which density of a halo is 500 times the cosmic critical density at the halo' s redshift). Assuming n_s and n_b are count rates of source and background, the signal-to-noise ratio can be calculated from:

$$\mathrm{S/N} = \frac{n_s}{\sqrt{n_s + n_b}}$$

Considering the criterion S/N > 10 and background count rate of HUBS, most hot baryons of a cluster can be detected if the source count rate in the 0.1-2 keV band at R_{500} meets n_s > 0.02 counts arcmin^{-2} s^{-1}.

On the other hand, before the PSF of HUBS is finally determined, we assume a cluster can be resolved as an extended source if it exhibits variation in the radial profile of X-ray luminosity. Based on the 1 arcmin^2 pixel size of HUBS and gas density profiles in model results (see results in Section 2.1 of Paper I and also Sharma et al. 2012), we assume a cluster to be an extended source if the angular diameter of its R_{500} radius is greater than 3 . Clusters with smaller angular size but S/N > 10 inside R_{500} are point-like sources that HUBS cannot resolve, but it is still possible for HUBS to detect hot baryons in these clusters with long enough exposure time.

In Figure 9 [Figure 9: see original paper], we show the redshift distribution per FoV of clusters with S/N > 10 inside R_{500}, averaged over the entire mock sky up to z = 1. The red curve is the number of extended sources, and the blue curve is the number of point-like sources unresolvable by HUBS. We can see that number density of resolved clusters at z = 0 is about 40 deg^{-2} in a redshift bin of Δz = 0.2. The value peaks at z 0.4 with almost 80 deg^{-2} per Δz and drops rapidly at z > 0.5 for decreasing angular size. Thus, survey of hot baryons in resolved clusters by HUBS should be effective below redshift 0.5 because of angular size of clusters in the soft X-ray band at different redshifts.

To test the redshift limit of resolved sources for HUBS, we select a massive bright cluster with L_X > 10^{45} erg s^{-1} at z 0.5 and show its mock observations in Figure 10 [Figure 10: see original paper]. Comparing the emissivity map of the cluster in Figure 4 and the photon-count image in the left panel of Figure 10, we see that the selected cluster is close to the angular resolution limit of HUBS. In the middle panel of Figure 10, the S/N map indicates that hot gas in the cluster at redshift around 0.5 can still be detected with an exposure time of 10^6 s, consistent with results in Zhang et al. (2022) that HUBS can detect groups and clusters beyond z 0.3. In addition, the mock spectrum in the right panel indicates it is also possible for HUBS to resolve strong emission lines in the bright cluster at z 0.5, and the flux rate of XRB photons is below 10^{-2} counts s^{-1} keV^{-1} (not plotted in Figure 10).

On the other hand, Figure 9 shows that the number of unresolved sources is around zero at $z = 0$ and increases with redshift. It exceeds the number of resolved clusters at $z > 0.3$ and reaches around 1000 deg^{-2} per Δz at $z > 0.8$. These unresolved sources are clusters with angular size below the angular resolution limit. Because of the large number of these point-like sources, hot gas in these clusters contributes a significant fraction of baryons at z 0.3. It is interesting to test mock observations of unresolved clusters. We select an unresolved cluster at z 1 with high signal-to-noise ratio. The halo mass M_{200} is around 3×10^{13} M , and its angular diameter of R_{500} is around 1.2 . After 10^6 s of observation by HUBS, about 8×10^4 photons can be detected in the 0.1-2 keV band. The mock spectrum of this cluster is shown in Figure 11 [Figure 11: see original paper]. Although the point-like source at z 1 is below the angular resolution limit, HUBS still has the ability to detect strong emission lines from such a source, such as O VIII and Ne X lines around 0.3 and 0.5 keV in the observed frame. It should be valuable to observe some sky areas with long exposure time to get signals from point-like sources of clusters at $z > 0.5$, which would help study properties and redshift evolution of hot baryons in the early universe.

In summary, by taking advantage of the large simulation box in SAMs, mock observation of HUBS will help in target selection and observation strategies for future surveys. Considering angular size of clusters, survey of hot baryons in resolved clusters by HUBS is effective below redshift 0.5. HUBS has the ability to detect emission lines of hot gas in clusters at $z > 0.5$, and observation of point-like sources with long exposure time can be used to study hot baryons in the early universe.

4. Summary

In this paper, we create mock X-ray observations of hot gas in galaxy clusters based on model outputs of a new extension of L-Galaxies SAMs from our recent work in Paper I.

First, we use coordinates and velocities in model outputs to build mock light cones up to nearby and deep redshifts. In each light cone, we use bolometric X-ray flux, gas temperature, and gas metallicity to generate mock X-ray spectra for galaxy clusters with the SOXS package, then derive mock X-ray images of each cluster based on spectra and projected X-ray luminosity profiles. Using mock data, we simulate X-ray spectra for the ROSAT all-sky survey and compare them with observational results. Then we consider design parameters of the HUBS mission and simulate observations of hot gas for HUBS to evaluate results for a future survey of hot baryons, which is an important application of our mock work.

The main conclusions are:

1. Our mock X-ray observations of hot gas can approximately match results from X-ray telescopes.
2. Due to angular size of clusters, survey of hot baryons in resolved clusters by HUBS is effective below redshift 0.5. HUBS has the ability to detect emission lines of hot gas in clusters at $z > 0.5$, and observation of point-like sources with long exposure time can be used to study hot baryons in the early universe.
3. Mock X-ray observations provide opportunities to select targets and optimize observation strategies for forthcoming X-ray facilities by taking advantage of the large simulation box and flexibility in SAMs.

This paper demonstrates applications of our mock data of hot gas, and many upcoming studies can be carried out in the future. One possible work is end-to-end simulation of the all-sky hot gas survey of HUBS and eROSITA considering various systematic and instrumental effects, such as background sources of AGNs, point-spread function, redistribution matrix file, etc., which provides source selection and detection functions at different redshifts. Another possible work is to create mock catalogs with SAMs outputs based on ELUCID (Wang et al. 2016), a constrained N-body simulation capable of reproducing spatial distribution of nearby galaxies and clusters in the real universe, and to simulate X-ray observations of clusters at given positions in the real sky.

In future SAMs work, it is also necessary to improve physical prescriptions of hot gas and X-ray emission, including X-ray emission from AGNs to improve scaling relations in bright clusters, cooling and feedback processes in inner haloes to improve density profiles in core regions of clusters, and also distribution of hot baryons beyond the halo virial radius R_{200}, which is proposed to be important for missing baryons in hydrodynamic simulations (e.g., Martizzi et al. 2019; Ayromlou et al. 2022).

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