The Young and the Wild: What Happens to Protoclusters Forming at Redshift $z \approx 4$?

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Abstract

Using one of the largest volumes of the hydrodynamical cosmological simulation suit Magneticum, we study the evolution of protoclusters identified at redshift $\approx 4$, with properties similar to the well-observed protocluster SPT2349-56. We identify 42 protoclusters in the simulation as massive and equally rich in substructures as observed, confirming that these observed structures can already be virialized. The dynamics of the internally fast-rotating member galaxies within these protoclusters resemble observations, merging rapidly to form the cores of the brightest cluster galaxies of the assembling clusters. Half of the gas reservoir of these structures is in a hot phase, with the metal enrichment at a very early stage. These systems show a good agreement with the observed amount of cold star-forming gas, largely enriched to solar values. We predict that some of the member galaxies are already quenched at $z \approx 4$, rendering them undetectable through measurements of their gas reservoirs. Tracing the evolution of protoclusters reveals that none of the typical mass indicators at high redshift are good tracers to predict the present-day mass of the system. We find that none of the simulated protoclusters at $z = 4.3$ are among the top ten most massive clusters at redshift $z = 0.2$, with some barely reaching masses of $M \approx 2 \times 10^{14} M_{\odot}$. Although the average star formation and mass growth rates in the simulated galaxies match observations at high redshift reasonably well, the simulation fails to reproduce the extremely high total star formation rates within the observed protoclusters, indicating that the subgrid models are lacking the ability to reproduce a higher star formation efficiency (or lower depletion timescales).

Unified Astronomy Thesaurus concepts: Early universe (435); Large-scale structure of the universe (902); High-redshift galaxy clusters (2007); Galaxy clusters (584); Computational methods (1965)

1. Introduction

Overdensities of galaxies at very high redshift have been observed in increasingly large amounts in the last few years, reaching redshifts as high as $z = 6$ and more. Assuming that those massive agglomerations of galaxies are the cores of structures that will collapse into very massive galaxy clusters at present day, these structures have been named protoclusters (see Overzier 2016, for an overview). Structures that will eventually collapse into a massive galaxy cluster by $z = 0$ are stretched out over several tens to hundreds of megaparsecs (e.g., Muldrew et al. 2015), and the galaxy overdensities that are observed thus are usually only the (possibly already collapsed) cores of these structures. On even larger scales, galaxy clusters are thought to collapse further into clusters of galaxy clusters, called super-clusters (Chon et al. 2014), until expansion freezes them in their positions in the cosmic web, counteracting gravity and thereby stopping the collapse of even larger modes.

Some of these observed protocluster cores reach masses high enough to challenge predictions from $\Lambda$-cold dark matter ($\Lambda$-CDM) cosmological simulations, for example the two massive protoclusters observed at $z \approx 4$, namely SPT2349-56 at $z = 4.3$ (Müller et al. 2018; Rotermund et al. 2021) with a total mass of more than $1 \times 10^{13} M_{\odot}$, and the even more massive protocluster reported by Oteo et al. (2018) at $z = 4.0$ with a total mass above $4 \times 10^{13} M_{\odot}$. Both of these protocluster cores have large numbers of member galaxies with extremely high total star formation rates of more than $6000 M_{\odot} \text{yr}^{-1}$. Even more challenging is the structure reported by Chanchaiworawit et al. (2019) at $z = 6.5$ with a virialized core mass of $M_{200} \approx 4.06 \times 10^{13} M_{\odot}$. Many more such overdensities at redshifts of $z = 4$ and higher have been recently reported (e.g., Ouchi et al. 2005; Toshikawa et al. 2012, 2014; Calvi et al. 2019; Harikane et al. 2019; Toshikawa et al. 2020; Calvi et al. 2021), with still large masses but not as extreme. Additionally, protoclusters are often associated with massive star-forming submillimeter galaxies (e.g., Zhang et al. 2022).

At lower redshift of about $z \approx 2$, several protocluster cores have been already observed. One of the first reported and by now best-studied protoclusters at this redshift is the so-called Spiderweb galaxy at $z = 2.16$ (Kurk et al. 2004; Zirm et al. 2008), which actually consists of several galaxies with extremely high star formation rates (Dannerbauer et al. 2014; Shimakawa et al. 2014, 2018), larger than what is reported for the star-forming main sequence at these redshifts (Santini et al. 2017; Pearson et al. 2018). Generally, extremely high star formation rates for both the whole protocluster core but also the individual galaxies in these cores have been confirmed for other protocluster cores as well from redshifts $4 < z < 2$ (e.g., Umehata et al. 2015; Kubo et al. 2016; Wang et al. 2016; Kubo et al. 2017; Wang et al. 2018), especially through observations of CO with the Atacama Large Millimeter/submillimeter Array (ALMA). Strazzullo et al. (2018) especially used CO observations of clusters at $z \approx 2$ to show that the star formation rates in these clusters are strongly enhanced compared to the field. However, while Aoyama et al. (2022) reported for their...
of the halo to good approximation. While many of the galaxies in such protoclusters seem to have enhanced star formation rates, some already quenched galaxies have also been reported. For example, Kubo et al. (2013) already reported a quiescent fraction of about 20%–50% in a protocluster region at \( z = 3.1 \), while McConachie et al. (2022) confirm even a quiescent fraction of 70% in a protocluster core at \( z = 3.37 \), and Shi et al. (2019) found an enhancement of quiescent galaxies in a protocluster structure at \( z = 3.78 \). A clear environmental dependence of the quenched fraction of galaxies can be already found around \( 3 < z < 2 \) (Kodama et al. 2007; Yonekura et al. 2022), and for redshifts between \( 1 < z < 2 \), quenched fractions have been shown to increase with lower redshifts in clusters (e.g., Cooke et al. 2019; Sarron & Conselice 2021) especially compared to the field (Cooke et al. 2019). The red sequence buildup is clearly apparent in galaxy clusters at \( z = 2 \) and below (Strazzullo et al. 2013, 2016; Hatch et al. 2017; Ando et al. 2022), suggesting that the agglomeration of red sequence galaxies could be good tracers for (proto)clusters at high redshift (Strazzullo et al. 2015), albeit detections of such quiescent galaxies are still rare above \( z = 3 \), see for example Kubo et al. (2021), but have now become accessible thanks to JWST (e.g., Nanayakkara et al. 2022). This is in agreement with simulations that report the morphology–density relation to be building up around \( z = 2 \) (Teklu et al. 2017).

From the simulation side, the evolution of galaxy clusters has been predicted to high redshift from models and dark-matter-only cosmological simulations so far (e.g., Chiang et al. 2013; Muldrew et al. 2015), as extremely large fully hydrodynamical cosmological simulations are expensive and thus still rare, but required to reproduce massive collapsed protoclusters at high redshift given that the formation of massive galaxy clusters requires the large modes of the power spectrum to be included in the simulation, although such modes can only be captured as long as they are smaller than the box size. However, zoom simulations of individual galaxy clusters have been used to study the star formation properties of protoclusters of galaxies (Bassini et al. 2020), but also especially the buildup of the cores of today’s most massive galaxies, the brightest cluster galaxies (BCGs) (Ragone-Figueroa et al. 2018; Rennenhau et al. 2020).

Given the large sizes of protoclusters, it is extremely difficult to map a full protocluster observationally, especially as determining the exact boundaries is impossible. Therefore, the terms protocluster and protocluster core as used in the observational literature usually denote not the full regions but rather the central parts of protoclusters. As we are using data from simulations in this work, we have the full 3D and evolution information for all our simulated structures, and thus we are not limited by the same restrictions and will stick to strictly physically motivated definitions. We will throughout this work use the following terminology:

1. Protocluster core: virialized\(^5\) halos identified in the simulations at a given redshift with masses above \( 10^{13} M_\odot \), as they are already bound structures with a common dark matter halo of such large mass that they are comparable to what is observed for protoclusters today in mass and will most likely be the center of a larger region that collapses into a galaxy cluster by present day. This is the region where also the central BCGs are forming.

2. Protocluster: the full region which comprised everything that will end up in the final structure at \( z = 0 \). While we call this a protocluster, we will see that some of the structures identified at high redshift as protocluster cores will end only as group-size halos and thus, technically, should be protogroups. However, we will call all such structures protoclusters here for the sake of clarity. Regarding technical aspects, such full regions are what we call a Lagrangian region.

3. Observed protocluster: associations of galaxies in close proximity observed at high redshift that are thought to be collapsing into galaxy clusters by present day.

Note that we will not attempt to find observed protocluster candidates here but rather select protoclusters by looking for their associated protocluster cores.

In this study, we will use one of the largest fully baryonic cosmological hydrodynamical simulation volumes from the Magneticum Pathfinder simulation suite, which we will introduce in Section 2, to identify for the first time protocluster core counterparts to those observed at \( z \approx 4 \) and study their properties in Section 3, including member star formation rates and quiescent fractions. Using the full power of the simulations, we will track those protocluster cores and their galaxies down to \( z = 0.2 \) in Section 4, also studying the impact of the cosmological parameters as well as the importance of simulation volumes in finding overdensities as massive as those currently observed, predicting maximum observable virialized masses up to \( z = 10 \). Finally, in Section 5, we will summarize and discuss the results.

2. The Magneticum Pathfinder Simulations

To find protoclusters at high redshift comparable to those observed recently in mass, a large fully baryonic simulation volume is required. For the major part of this study we use one of the largest volumes from the hydrodynamical cosmological simulation suite Magneticum Pathfinder\(^6\) (K. Dolag et al., 2023, in preparation), for which the resolution is high enough to resolve galaxies down to baryonic masses of \( M_{\text{bar}} > 10^{10} M_\odot \). This simulation, Box 2b (see Bouclet et al. 2016; Ragagnin et al. 2019; Kimmig et al. 2022), has a box size of \((640 \text{ Mpc}) h^{-1}\)^3 and a particle mass resolution of \( m_{\text{DM}} = 6.9 \times 10^5 M_\odot h^{-1} \) and \( m_{\text{Gas}} = 1.4 \times 10^5 M_\odot h^{-1} \) for dark matter and gas, respectively. Since each gas particle can spawn up to four stellar particles during its lifetime, the mass of a stellar particle is approximately \( m_\star \approx 3.5 \times 10^4 M_\odot h^{-1} \). For dark matter and gas particles the same softening is used, with \( \epsilon_{\text{DM}} = \epsilon_{\text{Gas}} = 3.75 \text{ kpc} h^{-1} \), while for the stars a softening of \( \epsilon_\star = 2 \text{ kpc} h^{-1} \) was adopted. For more details on this specific simulation and its clusters and galaxies at low redshift, see Remus et al. (2017), Lotz et al. (2019), Harris et al. (2020), and Lotz et al. (2021).

The Magneticum simulations adapt a Wilkinson Microwave Anisotropy Probe 7 (WMAP 7) \( \Lambda \)-CDM cosmology (Komatsu

\(^5\) Note that in simulations virialized structures are defined via a density contrast predicted from spherical top-hat models. The protocluster structures, however, are fast growing, so the virial ratio here also includes the surface term and should not be confused with being a static system. Nevertheless, the velocity dispersion of the member galaxies typically reflects the virial velocity of the halo to good approximation.

\(^6\) www.magneticum.org
et al. 2011), i.e., \( \sigma_8 = 0.809, \ h = 0.704, \ \Omega_m = 0.272, \ \Omega_b = 0.0451. \) For the initial slope of the power spectrum, a value of \( n_s = 0.963 \) is used. The simulation was performed with an updated version of GADGET-3, including, in addition to various modifications in the formulation of smoothed particle hydrodynamics (SPH; Dolag et al. 2004, 2005; Donnert et al. 2013; Beck et al. 2016), modernized versions of the subgrid physics, especially with respect to the star formation and metal enrichment descriptions (Tornatore et al. 2004, 2007; Wiersma et al. 2009), and the black hole (BH) feedback (Fabjan et al. 2010; Hirschmann et al. 2014). BHs are represented by collisionless “sink particles” that can grow in mass by the accretion of gas from their environments, following the Bondi–Hoyle–Lyttleton approximation (Hoyle & Lyttleton 1939; Bondi & Hoyle 1944; Bondi 1952), or by merging with other BHs. We assume that a small fraction of the radiated energy which goes in hand with the accretion is thermally coupled to the surrounding gas and deposited in form of heat. Additionally, we incorporated the feedback prescription to account for a transition from a quasar- to a radio-mode feedback whenever the BH is in a low accretion state, where we assume a significantly larger coupling efficiency to mimic the observed, mechanical feedback in this radio mode. For more details on the physics included in the Magneticum Pathfinder simulations, we refer the reader to Hirschmann et al. (2014), Teklu et al. (2015), and Dolag et al. (2017).

The data of these simulations up to redshift \( z \approx 2 \) are publicly available on the Cosmological Web Portal, see Ragagnin et al. (2017). In general, the main suite of the Magneticum simulations encompasses five different simulation volumes: Box 0 with a box length of \( (2688 \text{ Mpc} h^{-1})^3 \), Box 1 with a box length of \( (896 \text{ Mpc} h^{-1})^3 \), Box 2b with a box length of \( (640 \text{ Mpc} h^{-1})^3 \), Box 3 with a box length of \( (128 \text{ Mpc} h^{-1})^3 \), and Box 4 with a box length of \( (48 \text{ Mpc} h^{-1})^3 \), all adopting the same physics and cosmology as described above. In addition, the Magneticum simulations include a set of 15 simulations of the Box 1 volume with a resolution of \( 2 \times 1526^3 \) particles, adopting different cosmologies with varying \( \sigma_8, H_0, \Omega_m, \) and \( \Omega_b \). These simulations have been introduced by Singh et al. (2020).

For all simulations, structures are identified using a modified version of SUBFIND (Springel et al. 2001; Dolag et al. 2009), where the center of a halo is defined as the position of the particle with the minimum of the gravitational potential. The virial mass, \( M_{\text{vir}} \), is defined through the spherical overdensity as predicted by the generalized spherical top-hat collapse model (Eke et al. 1996). In particular, we use the fitting formulae presented in Equation (6) of Bryan & Norman (1998) to infer the virial overdensity when computing \( R_{\text{vir}} \) (and the associated \( M_{\text{vir}} \)) for halos in the simulations for the differed cosmologies.

### 3. Protocluster at \( z \approx 4 \)

As the recently detected massive observed protoclusters are at redshifts of about \( z \approx 4 \) (Miller et al. 2018; Oteo et al. 2018; Rotermund et al. 2021), we select our protocluster candidates at a similar redshift snapshot of \( z = 4.2 \). These observed protoclusters consist of several galaxies clustered in a very small volume. It is not known for sure from observations that such structures are already decoupled from the large-scale expansion, albeit it is very clear at least for the case of SPT2349-56 from the phase-space distribution of the galaxies (Miller et al. 2018) that they are already within a collapsed structure. Therefore, we select our protocluster candidates based on the total mass that is within the overdensity surface, corresponding to the predicted virial overdensity. This is found by applying the Friends-of-Friends algorithm (Davis et al. 1985), with a linking length of 0.16. At \( z = 4.2 \), this provides us with 42 candidates with total masses above \( M_{\text{tot}} = 1 \times 10^{13} M_\odot \).

However, this is not a possible detection criterion for observations, so we refine our selection criteria from this pool of protocluster candidates based on the following four methods that closely mimic observational methods: first, the galaxies in these observed protoclusters are in close vicinity and their velocities indicate that they are already bound to the main common potential (Miller et al. 2018). Therefore, it is a fair assumption that they can already be considered virialized. This provides the simplest of all identifications, namely by the virial mass of the halo, so we can rank our simulated protocluster candidates due to the virial mass of their cores. This results in ranking the protocluster candidates by their virial mass, and results in the most concentrated structures at that redshift. We find the most massive system to have a total mass of \( M_{\text{vir}} = 2.148 \times 10^{13} M_\odot \). Table 1 lists the 16 most massive bound structures in our simulation at \( z = 4.22 \) according to their total (virial) mass (upper part).

A second approach is to identify protoclusters based on an already very massive central galaxy (a protoBCG), with several smaller galaxies in close vicinity. The lower part of Table 1 lists the 16 protocluster candidates with the most massive stellar galaxy \( M_{\text{CD}} \). As can be seen immediately from this table, there is no direct correlation between the total mass of the protocluster candidates and the stellar mass of the most massive galaxy in the structure; in fact, only half of the structures with the highest total mass are present in the list of 16 structures with the most massive stellar components. This already indicates that there is no simple indicator that uniquely links the total mass growth and the growth of the stellar components at this epoch.

However, observationally the total (or dynamical) mass is difficult to measure, and structures at high redshift are usually detected due to their extreme luminosity indicative of high amounts of star formation, or due to their overdensity in number of galaxies. Therefore, with method 3 we also select 16 protocluster candidates as the most star-forming structures at \( z = 4.2 \) (see the upper part of Table 2). Interestingly, the structure with the highest star formation rate of \( 2858.06 M_\odot \cdot \text{yr}^{-1} \) is the second most massive structure in our simulation box, and the three most star-forming structures are all among the 16 most massive structures. However, similar to what we found for the stellar mass of the most massive galaxy, about half of the most star-forming structures are not among the most massive structures in our sample.

Additionally, we also select the 16 structures with the highest number of galaxies at \( z = 4.2 \) (see the lower part of Table 2), with the richest structure hosting 25 galaxies, all of which are star forming. This structure has, in fact, a total mass

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*References and notes*:

8. This value is obtained by scaling the canonical value of 0.2 (e.g., Efstathiou et al. 1988; Goetz et al. 1998) to the cosmology used in our simulation.

9. Here we use \( M_{\text{tot}} \), the density contrast calculated from the top-hat model. These values (and the ranking) will slightly change if we use \( M_{200\text{mean}} \) or \( M_{200\text{cent}} \).
of only $M_{\text{vir}} = 9.83 \times 10^{12} M_{\odot}$, and thus is definitely not among the 42 most massive structures in our simulation at $z = 4.2$. Here, we find the first very interesting tendency: from the 16 richest structures, only three are among the 16 most massive structures in our simulation box, clearly indicating that richness in member numbers is not a good tracer for the most massive structures at redshifts as high as $z = 4.2$.

### 3.1. Selecting a Set of Protoclusters at $z = 4.2$

From each of the four categories introduced above, we now choose a total of eight protocluster regions to study in more detail in this work, which we will call protoclusters (PCl) in the following and which are highlighted in gray in Tables 1 and 2: PCl0, PCl1, PCl2, PCl3, PCl4, PCl5, PCl7, and PCl12. Images of all these eight clusters can be seen in the upper-right panels of Figure 1, with each left panel showing the gas of the protocluster and its environment, and the right panel showing the stellar particles in the innermost 1329 kpc $h^{-1}$ comoving (which is 353.77 kpc physical at $z = 4.2$), centered around the protocluster core. In particular, those eight clusters were chosen as follows: PCl3, PCl12, PCl0, and PCl5 are the four protoclusters with the highest star formation rates, PCl1 also being among the 16 protoclusters with the highest star formation rates (rank 11); PCl5, PCl1, and PCl7 are the three richest protoclusters in terms of galaxy membership, with PCl0 also being among the 16 richest protoclusters (rank 12); PCl0, PCl12, PCl1, and PCl4, and PCl1 are the most massive protoclusters with respect to the total mass, with PCl12 being also among the 16 most massive ones (rank 7); finally, PCl14 is the structure with the most massive stellar galaxy, with the central galaxies of PCl1 and PCl12 also belonging to the 16 most massive central galaxies (rank 10 and 12, respectively). PCl1 is the only protocluster that is part of all four categories, and its innermost part is shown in the lower central panel of Figure 1 with both stars and gas, with gas rotation maps shown for four of its most gas-rich galaxy members. Interestingly, the properties of our PCl1 are strikingly similar to those found for SPT2349-56 (Miller et al. 2018; Rotermund et al. 2021): PCl1 has a BCG stellar mass of $M_{\text{CD}} = 5.7 \times 10^{11} M_{\odot}$, while the BCG...
1. The 16 highest-ranking protocluster candidates at $z = 4.2$ selected according to their total star formation rate (upper table block) and their total number of member galaxies $N_{\text{gal}}$ (lower table block).

found for SPT2349-56 has been reported to have $M_{\text{BCG}} = 3.2 \times 10^{11} M_{\odot}$; PCl 1 has 19 member galaxies above $M_{\text{gal}} > 10^{10} M_{\odot}$, whereas there are so far 14 member galaxies reported for SPT2349-56. And the total stellar mass reported for the central part of SPT2349-56 is about $M_{*} = 1.2 \times 10^{12} M_{\odot}$, while the total stellar mass in the virialized region of PCl 1 is $M_{*} = 9.3 \times 10^{11} M_{\odot}$. Gas rotation maps are also shown for two gas-rich galaxies from PCl 0, which satisfies three of our four protocluster candidate selection criteria.

The cold gas disks in those gas-rich galaxies found in our protoclusters are of similar gas masses as those observed at high redshift (e.g., Dannerbauer et al. 2017), and are typically all rotating at rather high velocities of about 200–600 km s$^{-1}$, which is slightly higher than the values reported from observations so far (Smit et al. 2018; Jones et al. 2021), albeit these observed galaxies are not inside protoclusters but rather identified due to their high UV luminosity, and thus they are not directly comparable to the galaxies inside the protoclusters shown in this work. As can be seen from the upper-left panel of Figure 1, all of the protoclusters sit at knots of the cosmic filaments, having already a heated atmosphere and accreted galaxies and mostly cold gas along the filaments, which penetrate deeply into the hot atmosphere. A detailed analysis of the hot atmosphere of these structures is outside the scope of this paper, where we will mainly focus on the properties of the galaxies and the growth of the structures; however, we will quickly discuss some aspects of this in Section 3.6. Still, as can be seen in the individual panels of Figure 1, the geometry of these clusters can be quite different, for example PCl 10 shows a quite striking linear geometry of the main member galaxies, while PCl 12 has a more spherical geometry.

3.2. Properties of the Galaxies within the Protoclusters at $z = 4.2$

The eight protoclusters selected from the simulation can clearly be classified as already bound systems. Note that by construction our selected protoclusters always have to be bound systems, and we can assume that the halo finding based on SubFind identifies all such systems in the simulations. Here, we do not intend to find systems which due to projection effects or observational uncertainties could be accidentally identified as spatially close and bound systems although they are not. However, as was shown already in Figure 1, some of our selected systems have the rather linear geometry of the main member galaxies, like PCl 10 but also PCl 1, clearly indicating active ongoing assembly, similar to what is observed for the
surroundings of the massive protocluster structures. Thus, comparing the phase-space distributions of the member galaxies from our simulated protoclusters to observations still provides important information about the comparability. Figure 2 shows the phase-space distribution of the member galaxies for the protocluster PCl 1 as an example. As can clearly be seen, the velocities of the individual galaxies, although many of them on first infall, are all smaller than the escape velocity. Interestingly, the distribution of the individual member galaxies within the phase-space in the simulated protocluster is actually very similar to the distribution reported for SPT2349-56 (Miller et al. 2018), again highlighting that PCl 1 is in fact a good match for SPT2349-56.

3.3. Star Formation and Quiescent Fractions in the Protoclusters at $z = 4.2$

For all our protoclusters we can also distinguish the star-forming from the quiescent galaxies. Following Franx et al. (2008), we use the specific star formation rate ($sSFR$), i.e., galaxies with $sSFR < 0.3 \times t_{\text{Hub}}$ are called quiescent, while galaxies with $sSFR > 0.3 \times t_{\text{Hub}}$ are classified as star forming.

3.3.1. Quiescent Fractions

As can be seen from Tables 1 and 2, about half of our eight example protoclusters (gray shaded) have no quiescent galaxies yet, while the other half host already one or two quiescent galaxies. Interestingly, the appearance of already quenched galaxies is not related to the virial mass of the system or the amount of member galaxies or the star formation rate. This becomes more evident when looking at all 42 protoclusters, as shown in Figure 3. Here, also no trend or correlation with the ranking of the protocluster according to the different selection criteria and the appearance of quiescent galaxies can be seen. For example, PCl 15, the protocluster with the highest number of galaxies, has no quiescent galaxy at all, while the protocluster with the largest number of quiescent galaxies, PCl 21, has only eight galaxies of which half are already quenched. This clearly shows that the quenched fraction at redshifts as high as $z = 4.2$
circles for the centers of mass of the member galaxies. In addition, black small dots mark the stars, blue small dots mark the cold gas particles, and cyan small dots are star-forming gas particles in the individual member galaxies. Black lines mark the escape velocity assuming a relaxed Navarro–Frenk–White halo for our protocluster PCL 1.

**Figure 2.** Comparison of the phase-space distribution of the galaxies within SPT2349-56 (pink open stars) and within our protocluster PCL 1 (red open circles for the centers of mass of the member galaxies). In addition, black small dots mark the stars, blue small dots mark the cold gas particles, and cyan small dots are star-forming gas particles in the individual member galaxies. Black lines mark the escape velocity assuming a relaxed Navarro–Frenk–White halo for our protocluster PCL 1.

**Figure 3.** Quiescent fraction for the 42 protocluster candidates vs. the four different tracers at $z = 4.2$ used to identify protoclusters: Upper left: quiescent fraction vs. virial mass. Upper right: quiescent fraction vs. stellar mass of the most massive member galaxy (BCG). Lower left: quiescent fraction vs. total star formation rate in the virialized region. Lower right: quiescent fraction vs. richness (number of member galaxies in the virialized region). The colored symbols mark the eight specific protoclusters as described in the text, with the colors green/cyan/blue/red/magenta/burgundy/dark blue/dark green marking PCl 3/12/0/5/1/7/2/4, respectively.

Figure 4. Average fraction of quiescent galaxies with redshift for Magneticum halos of different virial mass ranges, as indicated in the legend. Observations of individual clusters from Strazzullo et al. (2019) are included as circles, and the protocluster from McConachie et al. (2022) is shown as a diamond, with the color indicating the mass range of the observed halos compared to the simulated mass range. In addition, stacked mean quiescent fractions from the DETECTIFz algorithm from the REFINE survey from Sarron & Conselice (2021) are included as stars, split into two mass bins corresponding to the two lowest simulated mass ranges shown here (F. Sarron et al. 2023, in preparation).

As already demonstrated in earlier work (Lotz et al. 2019), our simulations generally reproduce the observed fraction of quenched galaxies well at $z = 0$ (Lotz et al. 2019) and at $z = 2.7$ (Lustig et al. 2023). Figure 4 shows the evolution of the quenched fraction depending on host halo mass for five different host halo mass ranges, from $z = 4.2$ to $z = 0.2$. As expected, the averaged quenched fraction within galaxy clusters (and groups) not only decreases with increasing redshift, but also decreases with halo mass at a fixed redshift. For galaxy clusters above $M_{\text{vir}} > 1 \times 10^{14} M_\odot$, the amount of quenched galaxies agrees well with observed quenched fractions from the SPT by Strazzullo et al. (2019) at redshifts up to $z = 1.72$, albeit our average quenched fraction is generally slightly lower than the observed values.

For the lower-mass end, we compare our results to observations from the DETECTIFz algorithm from the REFINE survey by Sarron & Conselice (2021). This extensive set of observations covers a redshift range up to $z \approx 2$, and the galaxy detection limit in stellar mass is at $M_* \approx 2 \times 10^{10} M_\odot$, in good agreement with what we can resolve in our simulations, which enables a comparison with respect to the relative quenched fractions. However, virial masses are not measured directly and need to be modeled, which is why the split into halo masses was done based on the stellar masses and not the halo masses, with the groups sorted into halo mass bins of $5 \times 10^{13} M_\odot < M_{\text{vir}} < 1 \times 10^{14} M_\odot$, being selected as having stellar masses of $M_* > 5 \times 10^{11} M_\odot$, and those that were sorted into the halo mass bin of $1 \times 10^{13} M_\odot < M_{\text{vir}} < 5 \times 10^{13} M_\odot$, being selected as having stellar masses of $1 \times 10^{11} M_\odot < M_* < 5 \times 10^{11} M_\odot$ (private communication, F. Sarron et al. 2023, in preparation).
be seen from the stars in Figure 4, the predicted quiescent fractions from the simulations are generally larger than what is observed for the group regime, albeit the lower-mass bin agrees reasonably within the error bars. Whether this is due to the split been made based on halo versus stellar mass, or due to other reasons is beyond the scope of this study.

At redshifts higher than \( z = 2 \), quiescent fractions are observationally extremely difficult to obtain. Here, we could only include one data point for the protocluster MAGAZ3NE-J0959 from McConachie et al. (2022) at \( z \approx 3.37 \), where the total halo mass is also only a rough estimate. Even though this protocluster has most likely a larger than average fraction of quiescent galaxies, it falls well within the upper 1\( \sigma \) range of our predicted quiescent fractions for halos of a total mass of \( 1 \times 10^{13} M_\odot < M_{\text{vir}} < 5 \times 10^{13} M_\odot \), indicating that our quenching mechanisms produce reasonable quenched fractions at high redshift, albeit it is only a single object to compare so far. Adding further observations to this will enhance our understanding of the relevant quenching mechanisms at high redshift in the future.

### 3.3.2. Star-forming Galaxies in the Protoclusters

One common finding regarding protoclusters is that models and simulations generally struggle to reproduce the large observed star formation rates (e.g., Saro et al. 2009 at \( z = 2 \); Granato et al. 2015 up to \( z = 3 \); Lim et al. 2021 up to \( z = 7 \)). In the left panel of Figure 5 we compare the observed integrated star formation rate as function of the area on the sky of SPT2349-56 from Miller et al. (2018) with our sample of eight selected protoclusters. While the BCGs of several of our protoclusters have a star formation rate which even exceeds the one of the most star-forming galaxy inside the observed protocluster, the sum of all the observed star formation rates within the same (virial) area is still a factor of \( \approx 3 \) larger than the one we find in the simulation for all our protoclusters, in agreement with the results found by Bassini et al. (2020) for zoom-in simulations of galaxy clusters.

On the other hand, comparing the amount of available gas between the observations and the simulations, as shown in the right panel of Figure 5, clearly shows that our protocluster candidates have very similar integrated cold gas mass values as the observations, and several of our protoclusters even exceed the observed gas mass values at all distances from the center. Even if we calculate the available gas only from what is inside the galaxy members of the protoclusters which (mostly) excludes the hot gas component, as shown as dashed lines in the right panel of Figure 5, some of the protoclusters still reproduce the observed values. Interestingly, the cluster closest in behavior to SPT2349-56 is again PCI1, with a nearly identical growth of cold gas mass with distance.

In general, this discrepancy between the observed and simulated star formation rates even though the observed and simulated cold gas reservoirs are in agreement and that is also reported for other simulations (e.g., Bassini et al. 2020) could have two reasons: either the simulations in general do not form stars efficiently enough to reproduce the observed values, or the stars are building up at this early times in a much more bursty way compared to the rather continuous rate at which stars are currently formed in simulations.

### 3.4. Stellar Mass Function at High Redshift

One clear test to answer the question whether simulations do generally not form stars efficiently enough is to check how the integrated star formation within the simulation compares to observations, i.e., to compare the stellar mass functions at different redshifts. For the Magneticum simulations, it has been shown by Hirschmann et al. (2014) and Steinborn et al. (2015) that the stellar mass function is generally well captured between \( z = 4 \) and \( z = 0 \), slightly overshooting the high-mass end at \( z = 0 \).

Figure 6 shows the stellar mass functions for Box 2b from \( z = 3.4 \) to \( z = 5.0 \). Given that (for data storage reasons) the spacing between the available outputs of the simulations is relatively large, comparisons with observations, which typically span certain ranges in redshifts, are more difficult. Therefore, in
the left panel of the figure we show the observations binned in the interval $z = 3-4$ as data points, compared to the simulation at $z = 3.4$. On one hand there is a good agreement at the high mass end, which is the important part for the protoclusters. On the other hand, however, the lack of handling AGN feedback in galaxies below a stellar mass of about $10^{10} M_\odot$ due to our resolution limit for the treatment of BHs clearly imprints in an overshooting of the stellar mass function at the low mass end, as a result of slight overcooling at the low mass end. The right panel compares the observations binned in the interval $z = 4-5$ with the simulation at $z = 4.2$ (blue line) and $z = 5.0$ (red line). Here, the judgment of the agreement between simulations and observations is more difficult, however, given the involved uncertainties in this comparison, the simulations seem to reasonably reproduce the observed stellar mass functions. In summary, we conclude that the description of the averaged star formation within the simulation seems to reasonably well match the real average star formation within the universe. Especially, the difference between the observed and simulated stellar mass functions are far smaller than the observed differences in the star formation rates. This again supports our speculation that the difference between the simulations and the observations with respect to the star formation rates at high redshift is caused by the fact that the simulations do not capture processes which lead to a locally, environment dependent higher star formation efficiency, and therefore the simulations are lacking the extreme star-bursting systems, while overall producing the right amount of stars.

3.5. Star Formation versus Gas Reservoir

The overall star formation of galaxies in the Magneticum simulations follows the observed main sequence of star-forming galaxies, both when expressed in terms of stellar mass and in the form of gas mass over a large range in redshift, as shown in the right panel of Figure 7. Therefore, the star formation rate within the galaxies overall are consistent with observations even at the redshifts of the protoclusters. However, the simulation fails to reproduce the population of extremely star-forming galaxies as observed in the protoclusters as well as the star-bursting systems (often classified as mergers) at $z = 2$ (e.g., Genzel et al. 2010).

On the other hand, as can be seen in the left panel of Figure 7, the star formation rates at a given gas mass are much lower than the observed ones, clearly quantifying the issue already seen from Figure 5, that the gas masses agree well with observations while the star formation rates at the same time are too low. This again indicates that it is not the general, averaged star formation description which is insufficient in the simulations but rather the simulations are not producing the short depletion times (or large star formation efficiencies) for systems in special conditions or environments. This results in the general stellar and gas masses fitting well with observations, but the individual star formation rates being too low.

Another quantity intricately connected to the stellar and gas masses as well as the star formation rate is the velocity dispersion in the gas disks where the star formation takes place. If the gas disks at high redshift are too turbulent compared to observations, with too large velocity dispersions, this could be another reason for the star formation rates to underperform. As can be seen from the upper panels of Figure 8, there are tight correlations in the simulations for the stellar masses and the velocity dispersions found for the stellar (left panel) and the cold gas (right panel) components, respectively, as well as between the velocity dispersions and the star formation rate, albeit the correlations between the masses and velocity dispersions is tighter than that found for the velocity dispersions of the components and the star formation rate.
forming galaxy HXMM05 at protocluster SPT 2349-56 at Guijarro et al. Genzel et al. 2018 SPT 2349-56 galaxies are shown with the same symbols. In addition, the value for the star-bursting galaxy CRLE at downward-pointing gray triangle, values from protocluster members from HELAISS02 (\(z = 2.5\)) are shown as gray squares, and member galaxies from the most distant spectroscopically confirmed overdensities z57OD (\(z = 5.7\)) and z66OD (\(z = 6.6\)) are shown as gray diamonds. Light gray lines show the power-law fits from Hubble Frontier Fields measurements (Santini et al. 2017).

While there are no observations of these correlations at redshifts as high as \(z = 4.2\), velocity dispersions of the cold gas have been observed at redshifts up to \(z = 2.3\), with predictions for high redshift from the trends found up to these redshifts (Übler et al. 2019). We included these observations in the right panels of Figure 8 for comparison of the general trends found for the correlation between the cold gas velocity dispersions and the stellar masses of the galaxies (upper panel) and the star formation rates (lower panel). Both simulations and observations show a correlation between all three quantities with a similar slope, and a general tendency for the gas velocity dispersions to be higher at higher redshift. Thus, as far as this comparison is possible, we find general agreement in the trends seen from observations and simulations, however, the absolute velocity dispersions seem to be generally higher than the expected values from the extrapolations of the observations, as indicated by the solid black line in the upper-right panel of Figure 8. Such enhanced velocity dispersions are generally seen for simulations even down to redshifts of \(z = 0\), see van de Sande et al. (2019), and is most likely a result of the differences in particle mass between dark and baryonic masses and the different softenings used for different particle types used in the currently available cosmological simulations (Ludlow et al. 2020), and most prominent for disk galaxies (Ludlow et al. 2021). How this affects the star formation properties of galaxies in protocluster environments needs to be studied in the future in more detail.

### 3.6. Intracluster Medium Properties at \(z = 4.2\)

So far, we have discussed the properties of the cold gas component of the galaxies found in the protoclusters, however, the buildup of the hot gaseous halo found in galaxy clusters at present day is already taking place in protoclusters at high
Figure 9. Properties of the gas inside the virial radius of protocluster PCI 1 at $z = 4.2$. Left panel: phase diagram where blue dots are the hot ICM phase. Black diamonds mark the small subset of the hot ICM which is already chemically enriched above 10% of the solar value. Right panel: histogram of the chemical enrichment of the cold (blue) and hot (red) phase of the gas.

redshift. As an example of the expected state of the gas within protoclusters at $z = 4.2$, the left panel of Figure 9 shows a phase diagram of the gas within the virial radius of protocluster PCI 1. At this point, roughly half of the baryonic material within the protocluster is still in the cold phase, which is partially star forming. The other half is already in a hot atmosphere, virialized with temperatures centered around ≈1 keV. The presence of gas with temperature of several keV clearly indicates the presence of merger shocks due to the fast growing structures. While the cold and star-forming gas is already largely enriched around solar values, the hot intracluster medium (ICM) is still mainly metal poor, and only ≈2% is already enriched above 10% of the solar abundance. The metal-enriched hot gas is generally in denser parts of the hot halo, as marked by the black diamonds in the left panel of Figure 9. Based on very similar simulations, Biffi et al. (2017, 2018) demonstrated that some gas which is in the ICM of present-day clusters was already enriched to solar metallicity at high redshift. This indicates that—as expected—some of the cold, very metal-enriched gas within the protoclusters will be heated by subsequent feedback and stays within the ICM until present time. Furthermore, this indicates that it could generally be possible to detect these protoclusters already at $z \approx 4$ in X-ray measurements.

4. Galaxy Cluster Evolution from Protoclusters to Present Day

Spectacular protocluster cores like SPT2349-56 are often speculated to be the progenitors of today’s most massive galaxy clusters. In the following we will use the power of the simulations and trace the previously identified protoclusters to $z = 0.2$.

4.1. Cluster Mass Evolution

While protoclusters surely present very large overdensities at high redshift, the complicated merging process which is involved in the formation of the most massive structures in the universe leads to a large uncertainty for matching the most massive structures appearing at high redshift to the most massive structures observed at present time. To illustrate this point, Figure 10 shows the growth of structures in the simulations in comparison with observations at various redshifts. The dark gray band marks the range of virial masses of the 10 most massive systems in the simulations at the different times and which very nicely encompasses the observations at various redshifts, indicated by filled symbols in that figure.

The colored lines show the individual evolution pathways of the eight example protoclusters. Interestingly, none of them is among the 10 most massive systems at redshift $z = 0.2$. Some of them even barely reach masses in the galaxy cluster range, and end up as very-low-mass cluster systems, like PCI 12 with a final mass of less than $2 \times 10^{14} M_\odot$. Some of the most massive clusters at $z = 0.2$ from our sample of eight protoclusters are actually below a virial mass of $1 \times 10^{13} M_\odot$ at $z = 4.2$, and thus in terms of virial mass below the threshold of what would be considered a protocluster (PCI 1 and PCI 7), i.e., they are only protoclusters if the total linked mass $M_{\text{tot}}$ is considered. From those protoclusters at $z = 4.2$ that are the most massive, only PCI 0 ends up as one of the most massive clusters, although our SPT2349-56 counterpart PCI 1 also reaches a final mass larger than $1 \times 10^{15} M_\odot$. Generally, from the 29 galaxy clusters with total masses larger than $1 \times 10^{15} M_\odot$ at $z = 0.2$, only seven actually have progenitors that are identified as protoclusters at $z = 4.2$, see Kimmig et al. (2022).

The weakness of the connection between the ranking of high-mass systems at high redshift with the ranking of the final system mass can also be clearly seen from Tables 2 and 1 and the upper-left panel of Figure 11. Furthermore, Figure 11 also shows that there is no correlation between the final mass of a cluster at $z = 0.2$ and either the stellar mass of the most massive galaxy, or the total star formation rate of the protocluster members. The only quantity for which we find a slight tendency to indicate the outcome of the mass evolution of a protocluster is the richness of the protocluster (see lower right panel of Figure 11), namely the number of galaxies that are part of the protocluster at $z = 4.2$. This is further supported by what can be seen from Tables 1 and 2, namely that the only selection
of the 15 most massive galaxy clusters in Magneticum
massive ones at the striped area shows the prediction from Chiang et al. at the redshift $z$.

The virial radius at $z=0.2$ is $\approx 5 \text{ Mpc}$. The stellar components of all galaxies present at $z=0.2$ have assembled half of their mass only since $z=0.6$ through recent merging of multiple groups and clusters, being the opposite of starved protoclusters, i.e., late assemblers.

4.2. Forming the BCG and the Intracluster light

As shown in the left panel of Figure 13, the BCG of our example protocluster PCI 1 (black line) grows very rapidly by three orders of magnitude between $z=7$ and $z=4$, while at redshifts below $z \approx 1$–2 the BCG grows much slower than the halo (gray line). The stellar components of all galaxies present within the virial radius of the protocluster at $z=4.2$ are already nearly completely merged into the BCG (solid red line) at the next available snapshot at $z=3.4$, and only a very minor stellar component (dashed red line) stays either as satellites or as stripped material within the system toward lower redshift. This is true for all our eight protocluster candidates, as shown in the

Figure 10. Total cluster mass vs. redshift. The colored lines show the evolution of the protoclusters selected at $z=4.2$, with colors green/cyan/blue/red/magenta/burgundy/dark blue/dark green marking the eight different example protoclusters PCI 3/12/0/5/1/7/2/4, respectively. The gray shaded area marks the mass range of the 15 most massive clusters in Magneticum Box 2b at each redshift, clearly showing that none of the protoclusters selected at $z=4.2$ is among the most massive ones at $z=0.2$. Gray filled circles show the SPT clusters taken from Miller et al. (2018), while the black stars show individual protoclusters selected with X-ray or optical methods taken from Miller et al. (2018) with additional points for SPT-CLJ1008-5844 at $z=1.132$ from Kim et al. (2019), the Spiderweb protocluster core at $z=2.16$ from Shimakawa et al. (2014), SSA22 at $z=3.09$ from Kabo et al. (2016), the Distant Red Core protocluster at $z=4.002$ from Oteo et al. (2018), and RO-1001 at $z=2.91$ from Daddi et al. (2021). Furthermore, the masses and redshifts of the structures from ORELSE by Tomczak et al. (2017) are shown as dark green symbols, and the values for the HYPERION group of merging protoclusters at $z \approx 2.45$ from Cucciati et al. (2018) are shown as light-green symbols. In addition, the striped area shows the prediction from Chiang et al. (2013) from the Millennium simulation in combination with a semi-analytic model (SAM).
right panel of Figure 13, and in good agreement with the results found by Rennehan et al. (2020). This clearly indicates a very short timescale on which these galaxies within the protocluster will merge at this redshift. This timescale is significantly less than 0.42 Gyr, which is the time span between the stored snapshots, thus it is not possible to obtain more information on the merging processes from the simulation but the simple fact that the merging takes places. Tracing the stellar component further in time reveals that, as expected, these stars that were already part of the protoclusters at \(z = 4.2\) mostly end up as part of the present-day BCGs, therefore effectively building up the cores of the present-day BCGs. Interestingly, as nearly all of the stars of these assembling galaxies end up in the BCGs, there is nearly no contribution to the intracluster light (ICL) component observed at present day, i.e., the extended diffuse stellar halo of the BCG, originating from the cluster formation phase at high redshift.

### 4.3. Effect of Cosmology and Simulation Volume

Finally, we evaluate the expected mass of the most massive structures at different redshifts, depending on the underlying cosmology. It is already well know that the cosmological parameters are closely correlated to the resulting halo mass functions, especially at the high-mass end and with respect to \(\sigma_8\) and \(\Omega_m\) (e.g., Abdullah et al. 2020). However, here we are especially interested in the impact of the cosmological parameters on the appearance of protoclusters at high redshift. Therefore, we use a new extension of the Magneticum simulation set as presented by Singh et al. (2020). These are resimulations of Box 1a, which has a volume of \((896 \, h^{-1} \text{Mpc})^3\), with \(2 \times 1526^3\) particles, using 15 different cosmologies by varying \(\sigma_8, \Omega_b, H_0\), as well as \(\Omega_m\). The cosmological parameters for the different runs are listed in Table 3. All simulations are run on the lowest available resolution (\(n_{\text{tr}}\)), with a particle resolution of \(m_{\text{DM}} = 1.3 \times 10^{10} M_\odot \, h^{-1}\) and \(m_{\text{Gas}} = 2.9 \times 10^9 M_\odot \, h^{-1}\) for dark matter and gas, respectively. For details see Singh et al. (2020).

Although these simulations follow the same hydrodynamical treatment and subgrid physics description as the simulation used for the previous part of this study, they have significantly less resolution and therefore we cannot perform a detailed analysis of protoclusters as done before with the much higher resolution simulation of Box 2b. Nevertheless, the resolution is high enough to predict the expectation of the most massive virial mass as a function redshift, similar to the upper limit of the gray shaded area in Figure 10. The colors are the same as used by Singh et al. (2020), and were originally chosen to go from low \(\Omega_m\) (blue) to a high value of \(\Omega_m\) (red). Due to choosing the cosmological parameters to follow the current observational constrains within the different figures of merit (for details see Singh et al. 2020), this means that the different values have nontrivial relationships and therefore it is impossible to construct a strict hierarchy of the models. As can be seen from left panel of Figure 14, the absolute mass of the most massive clusters at high redshift depends mostly on the value of \(\sigma_8\), i.e., the larger \(\sigma_8\) the more massive structures appear already at high redshift, as can be seen especially from the runs C3 (turquoise line) and C13 (orange line). Effectively, this results in a different slope for the highest mass per redshift relation, with flatter slopes for larger values of \(\sigma_8\). There is only a small trend with \(\Omega_m\), with larger \(\Omega_m\) producing larger...
structures at a given redshift, but this trend is only of secondary order. This clearly shows that measuring the most massive structures present at different redshifts can set constraints on the values of $\sigma_8$, and thus protoclusters might be usable as cosmological probes.

Furthermore, we can also see the effect of the different volumes of the simulated boxes from the left panel of Figure 14, where the solid black line marks the most massive halos per redshift for the smaller but higher resolved simulation Box 2h, in comparison to the black dashed line that marks the Box 1a cosmological run (C8) with the same cosmology as the Box 2b simulation used for most of this work. The low-resolution simulation of Box 1a (dashed line) has roughly three times the volume of the high-resolution simulation Box 2b (solid line), showing a mild trend to harbor larger structures, as expected due to the larger cosmological modes included in the larger simulation volumes, independent of the resolution. This is also further highlighted in the right panel of Figure 14, where the most massive structures per redshift are shown for all five volumes that are part of the Magneticum Pathfinder simulation suite (with the same cosmology as Box 2b). The smaller box volumes of Box 4 and Box 3 with box lengths of $(48 \text{ Mpc}/h)$ and $(128 \text{ Mpc}/h)$, respectively, are too small even to include collapsed structures with masses above $10^{13} M_\odot$ at $z = 4$, although they have the same cosmology and physics as the larger boxes which are large enough to capture the modes of the power spectrum that are responsible for growing the extremely large structures. This clearly demonstrates the need for large enough box volume simulations to capture those massive protoclusters that are now detected at high redshift and study their properties and evolution pathways.

### 4.4. Predictions to $z = 10$

Finally, we extend our study of the most massive already bound systems with redshift toward even higher redshifts of $z = 10$, the highest redshift at which already bound halos with stellar components can be found in the simulations given the resolution limits. We predict that halo masses of up to $M_{\text{vir}} = 1 \times 10^{12} M_\odot$ can already be found at $z = 9$, as shown in Figure 15, and a few times $10^{11} M_\odot$ at $z = 10$. As can also be seen, the massive protocluster at $z = 6.5$ presented by Chanchaiworawit et al. (2019) has a mass larger than any of our simulations, even the largest simulation volume, can reproduce, albeit the error bars are rather large. Whether this indicates that none of our simulation volumes is large enough to capture such massive structures, if that particular object is an outlier, or if the mass could be overestimated is beyond the
resolution, while Box 4

protocluster from Chanchaiworawit et al.

from observations by Shimasaku et al.

lower-mass protoclusters at

from Calvi et al.

described in Figure 10 with the addition of the high redshift

Box 2b

et al. (2020). Star symbols mark all individual (proto)cluster observations from Figure 10, with the addition of the $z = 6.5$ protocluster from Chanchaiworawit et al. (2019) and the protocluster at $z = 5.2$ from Calvi et al. (2021). Furthermore, a compilation of lower-mass protoclusters at $z > 4.8$ courtesy of F. Sinigaglia is added, sampled from observations by Shimasaku et al. (2003), Venemans et al. (2004), Ouchi et al. (2005), Toshikawa et al. (2012, 2014), Higuchi et al. (2019), and Toshikawa et al. (2020). Right panel: same as left panel but for the five different box volumes of the Magneticum Pathfinder simulation suite with the same cosmology. Box 0 (2688 Mpc $h^{-1}$) and Box 1 (896 Mpc $h^{-1}$) are performed with the lowest resolution, Box 2b (640 Mpc $h^{-1}$) and Box 3 (128 Mpc $h^{-1}$) are performed on high resolution, while Box 4 (48 Mpc $h^{-1}$) is on the highest available resolution.

\begin{figure}
\centering
\includegraphics[width=0.45\textwidth]{Figure14a}
\includegraphics[width=0.45\textwidth]{Figure14b}
\caption{Left panel: similar to Figure 10, but comparing the observations to the virial mass of the most massive systems from the 15 simulations with different cosmologies (see Table 3) at each redshift. Color coding is according to the value of $\sigma_v$. For the detailed parameters of the models, see Singh et al. (2020). Star symbols mark all individual (proto)cluster observations from Figure 10, with the addition of the $z = 6.5$ protocluster from Chanchaiworawit et al. (2019) and the protocluster at $z = 5.2$ from Calvi et al. (2021). Furthermore, a compilation of lower-mass protoclusters at $z > 4.8$ courtesy of F. Sinigaglia is added, sampled from observations by Shimasaku et al. (2003), Venemans et al. (2004), Ouchi et al. (2005), Toshikawa et al. (2012, 2014), Higuchi et al. (2019), and Toshikawa et al. (2020). Right panel: same as left panel but for the five different box volumes of the Magneticum Pathfinder simulation suite with the same cosmology. Box 0 (2688 Mpc $h^{-1}$) and Box 1 (896 Mpc $h^{-1}$) are performed with the lowest resolution, Box 2b (640 Mpc $h^{-1}$) and Box 3 (128 Mpc $h^{-1}$) are performed on high resolution, while Box 4 (48 Mpc $h^{-1}$) is on the highest available resolution.}
\end{figure}

\begin{figure}
\centering
\includegraphics[width=0.45\textwidth]{Figure15a}
\includegraphics[width=0.45\textwidth]{Figure15b}
\caption{Similar to Figure 10, but extended as predictions of the highest expected total masses to be found up to redshifts of $z = 10$, using the two largest box volumes from the Magneticum Pathfinder suite of simulations at low Box 0 (2688 Mpc $h^{-1}$) and high Box 2b (640 Mpc $h^{-1}$) resolutions. For Box 2b, at each redshift the mass range of the 10 most massive systems is shown as the gray shaded area, while for Box 0 only the line for the most massive system per redshift is shown. A compilation of observed systems as described in Figure 10 with the addition of the high redshift $z = 6.5$ protocluster from Chanchaiworawit et al. (2019) and the protocluster at $z = 5.2$ from Calvi et al. (2021) is shown as blue stars. Furthermore, a compilation of lower-mass protoclusters at $z > 4.8$ courtesy of F. Sinigaglia is added, sampled from observations by Shimasaku et al. (2003), Venemans et al. (2004), Ouchi et al. (2005), Toshikawa et al. (2012, 2014), Higuchi et al. (2019), and Toshikawa et al. (2020).}
\end{figure}

5. Discussion and Conclusion

Utilizing the very large cosmological hydrodynamical simulation Box 2b of the Magneticum project, which includes a subresolution treatment of star formation and stellar evolution, and a treatment of the effect of supermassive BHs, we show that such simulations, once the volume is large enough, can successfully produce massive protoclusters like SPT2349-56, reproducing many of their physical properties. Especially, we find several virialized structures at $z = 4.2$ with a similar number of member galaxies (richness) and the same dynamical properties of the member galaxies as the observed protocluster SPT2349-56 at $z = 4.3$ (Miller et al. 2018; Rotermund et al. 2021), but also similar to the protocluster core found by Oteo et al. (2018) at $z = 4$. The simulations also predict that several of the member galaxies of these structures are fast-rotating systems, in agreement with the observed findings for member galaxies of SPT2349-56.

We find that these member galaxies at $z = 4.2$ will merge on very short timescales, forming the progenitors of today’s cluster BCGs, in agreement with results found by Rennehan et al. (2020). The stellar component merging from these satellite galaxies assembles to build up the core of the BCG, and indicating that the centers of today’s massive BCGs echo this fast growing phase and their central velocity dispersion may reflect the dynamics of the galaxies within these protoclusters, being significant smaller than the velocity dispersions of the present-day clusters in which the BCGs live (see Bender et al. 2015; Remus et al. 2017; Sohn et al. 2020).

However, while the general stellar and total masses of the simulated protoclusters and the number and dynamics of member galaxies within resemble the observations closely, the instantaneous integrated star formation rates within such simulated protoclusters are a factor $\approx 2$–3 smaller than the observed values, although the simulations are reproducing the observed integrated gas mass within the protoclusters. As the simulations also reasonably well reproduce the main sequence of star-forming

scope of this work, but will be interesting to investigate in the future. All other systems reported at redshifts above $z = 4.2$ are well within the predicted mass range from our simulation.
galaxies as well as the observed stellar mass function up to this redshift, this indicates that the star formation in the simulations lacks the ability to reproduce higher star formation efficiency (or accordingly lower depletion timescales) at least in certain environments. The reason for this issue can be found most likely in the implementation of the star formation process that currently assumes a rather continuous star formation and a Schmidt–Kennicutt relation that holds true even at high redshift, an issue that needs to be addressed in future simulations.

While star-forming galaxies are detectable in the high-redshift protoclusters due to their large gas reservoirs, the quiescent galaxies at high redshift are much more elusive. Using our sample of 42 simulated protoclusters, we find that there can already be quenched galaxies in such protoclusters, albeit their number is low, and on average barely 10% of the total mass range of such protoclusters (around $10^{13} M_\odot$). Their quiescent fractions do not depend on the dynamical state of the protocluster, neither its virial mass, nor the overall star formation rate, nor the richness. We compare our quiescent fractions to observations at lower redshift where quiescent fractions can actually be inferred (Strazzullo et al. 2019; Sarron & Conselice 2021), and find an overall agreement, in agreement with previous work done by Lotz et al. (2019, 2021). We find the quiescent fraction to increase generally strongly with decreasing redshift, even at a fixed total mass, clearly showing that quenching becomes more efficient at lower redshift in both group and cluster environments.

The simulations predict that the star-forming gas in protoclusters at redshifts of $z \approx 4$ is already enriched to roughly solar values. Part of this cold gas is expected to be subsequently heated by feedback and become part of the ICM of the forming galaxy cluster. About half of the gas within these structures at $z = 4.2$ is already significantly heated to temperatures around 1 keV, and a very small fraction ($\approx 2\%$) of this hot gas is already enriched to one tenth of the solar value.

Using the full power of the simulation, we traced the protoclusters identified at $z = 4.2$ down to $z = 0.2$, to test the hypothesis that the extremely massive structures found at high redshift really are the progenitors of the most massive galaxy clusters at present day. However, at $z \approx 4$, these protocluster regions reflect only a very minor part of the Lagrangian region which will collapse into the final galaxy clusters at $z = 0.2$, and therefore none of the protocluster properties at $z = 4.2$ (e.g., virial mass, star formation rate, stellar mass, or richness in members) proves to be a good proxy for the mass of the final cluster at $z = 0.2$. In fact, from our eight examples chosen to be a among the top in these measures at $z = 4.2$, none is among the 10 most massive clusters at $z = 0.2$. Even more striking, one of them evolves barely into a very-low-mass cluster with a virial mass of less than $1 \times 10^{14} M_\odot$. From the full sample of 42 protoclusters at $z = 4.2$, four do not even grow above a mass of $1 \times 10^{14} M_\odot$. This is due to the fact that nodes in the cosmic web can collapse at very different timescales, and some of the nodes that collapse rather early starve and become fossil systems. Moreover, for the same simulation it was also shown recently that from the 29 most massive galaxy clusters at low redshift only seven are among our protocluster sample, and about a third of these massive galaxy clusters have assembled half of their mass only recently, i.e., since $z = 0.6$ (Kimmig et al. 2022). This indicates that not only do some nodes starve, but also some of the most massive nodes only collapse so late that they do not show a significant signal at redshifts as high as $z = 4.2$. With respect to the observable quantities within protoclusters at high redshift, we find the richness in galaxy members to be the only quantity that has a slight indication for the future of the system, in that rich systems tend also to evolve into massive systems at $z = 0.2$; however, the opposite is not true as also some systems that are low in richness at $z = 4.2$ evolve into massive clusters at present day.

Utilizing a second set of simulations from the Magneticum Pathfinder suite of simulations, which were performed with 15 different cosmologies (Singh et al. 2020), we quantified the expected largest mass of bound systems with redshift. Given the current uncertainties in the actual values of the cosmological parameters, we showed that the highest mass per redshift is actually a good tracer for $\sigma_8$, with the discrepancies larger the higher the redshift. Thus, finding the most massive bound systems at high redshift can set constraints on those cosmological parameters.

To conclude, we found that, on one hand, various aspects of observed protoclusters can be successfully reproduced by current state-of-the-art cosmological simulations if the simulation volumes are large enough. These protocluster structures have already virialized cores, already hosting a significant hot atmosphere which could be targeted observationally. On the other hand, detailed comparisons of the star formation rates reveal, as indicated in previous work from various simulation suites, that there seems to be some environmental increase in the star formation efficiency (or accordingly reduced depletion timescales) which current subresolution models describing the star formation within the simulations are not able to capture, albeit gas masses and both the general star formation main sequence and the stellar mass functions are reproduced successfully. While some of the protocluster systems found at $z \approx 4$ evolve into massive clusters at $z = 0.2$, they are not among the progenitors of today’s most massive clusters, and some of them barely reach cluster masses. Overall, the simulations shape a picture of a fast growing mode of massive systems at early time, which should still be echoed in the dynamical properties of the central parts of today’s massive BCGs, with a broad range of outcome in total mass at low redshift.

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