The velocity structure of the intracluster medium during a major merger: Simulated microcalorimeter observations

Veronica Biffi\textsuperscript{1,2}, John A. ZuHone\textsuperscript{2}, Tony Mroczkowski\textsuperscript{3}, Esra Bulbul\textsuperscript{4}, and William Forman\textsuperscript{2}

\textsuperscript{1} INAF – Osservatorio Astronomico di Trieste, Via Tiepolo 11, 34143 Trieste, Italy  
e-mail: veronica.biffi@inaf.it  
\textsuperscript{2} Center for Astrophysics, Harvard & Smithsonian, 60 Garden St., Cambridge, MA 02138, USA  
\textsuperscript{3} ESO – European Southern Observatory, Karl-Schwarzschild-Straße 2, 85748 Garching, Germany  
\textsuperscript{4} Max-Planck-Institut für Extraterrestrische Physik, Gießenbachstraße 1, 85748 Garching, Germany

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ABSTRACT

Major mergers between galaxy clusters can produce large turbulent and bulk flow velocities in the intracluster medium (ICM) and thus imprint useful diagnostic features in X-ray spectral emission lines from heavy ions. As successfully achieved by Hitomi in observations of the Perseus cluster, measurements of gas velocities in clusters from high-resolution X-ray spectra will be achievable with upcoming X-ray calorimeters such as those on board XRISM, Athena, or a Lynx like mission. An interesting application to clusters involves detecting multiple velocity components or velocity gradients from diagnostic observations of specific interesting locations across the cluster. To explore this possibility in the case of a major head-on cluster merger, we performed velocity analyzes of a cluster-cluster merger from a hydrodynamical simulation by means of X-ray synthetic spectra with a spectral resolution on the order of a few eV. We observed the system along two extreme line-of-sight directions: (1) perpendicular to the plane of the merger and (2) along the merger axis. In these geometrical configurations, we found that clear non-Gaussian shapes of the iron He-like Kα line at 6.7 keV are expected. While the velocity dispersion predicted from the simulations can be retrieved for the brightest 100 ks pointings with XRISM Resolve, some discrepancy with respect to the expected value is noted and can be attributed to the complex non-Gaussian line shapes. Measurements in low surface brightness regions, especially when multiple velocity components are present along the line of sight, require high signal-to-noise ratio and the larger collecting area of the Athena X-IFU calorimeter is therefore required. With the latter, we also investigated the ICM temperature and velocity gradient across the merger bow shock edge, from 20\textdegree-wide annuli extracted from a single 1 Ms X-IFU observation. For both temperature and velocity dispersion, we found best-fit values that are consistent with predictions from the simulations within 1\sigma. The uncertainties on the inferred velocity dispersion are, however, too large to place any stringent constraints on the shallow gradient downstream of the shock. Additionally, we present simulated images of the thermal and kinetic Sunyaev–Zeldovich effects from this merging system, using the above viewing configurations and compare the results at angular resolutions appropriate for future observatories such as CMB-S4 and the Atacama Large Aperture Submillimeter Telescope (AtLAST).

Key words. galaxies: clusters: intracluster medium – X-rays: galaxies: clusters – methods: numerical

1. Introduction

The diffuse intracluster medium (ICM) in galaxy clusters retains a wealth of information about the interaction with member galaxies, energetic feedback processes from stellar sources and black holes, chemical enrichment, and the system accretion history and merging events with other groups and clusters of galaxies. All these processes not only leave an imprint on the thermal structure of the ICM, but also exhibit kinematic signatures. The velocity diagnostics of the ICM therefore provide a complementary picture of cluster physics (Simionescu et al. 2019) to the thermal and chemical diagnostics. Gas motions of nonthermal origin, driven for instance by accreting streams of gas from filaments, or in the form of motions caused by infalling substructures and mergers (Lau et al. 2009; Fang et al. 2009; Biffi et al. 2011; Nagai et al. 2013; ZuHone et al. 2016a; Baldi et al. 2017), are crucial to measure because they can provide substantial additional pressure support to the system. This, in turn, can bias X-ray and Sunyaev–Zeldovich (SZ) mass estimates based on the assumption of hydrostatic equilibrium (HE; e.g., Pratt et al. 2019), as investigated by several simulation studies (Rasia et al. 2006; Nagai et al. 2007; Meneghetti et al. 2010; Suto et al. 2013; Lau et al. 2013; Nelson et al. 2014; Shi et al. 2016; Biffi et al. 2016; Oppenheimer 2018; Vazza et al. 2018; Pearce et al. 2020; Angelinelli et al. 2020; Gianfagna et al. 2021).

Even though residual gas motions can be present in relaxed clusters as well, they are particularly important in disturbed systems. In fact, cluster mergers can develop significant bulk motions in the ICM, with large gas velocities up to thousands of km s\(^{-1}\) (e.g., Dupke & Bregman 2005; Simionescu et al. 2019). Furthermore, disturbances of the ICM velocity field can also persist after the merging event, contributing to a deviation from HE (Nelson et al. 2012, 2014; Ghirardini et al. 2018). If, on the one hand, merging systems are evidently not suitable for measuring HE-based masses, they provide, on the other hand, the possibility to measure large gas velocities and map the velocity field to constrain the merger state and geometry. Observations have already singled out many systems showing clear signatures of merging activity, including extreme examples. These include cases where the merging occurs in (or close to) the plane of the sky, as well as galaxy clusters
merging along the line of sight (l.o.s.) direction, as suggested for instance from multiple peaks in the redshift distribution of their galaxies or from the central off-set between the galaxy spatial distribution and the X-ray emission. Mergers in the plane of the sky include well-known systems such as the Bullet cluster (Markevitch et al. 2002), A3266 (De Grandi & Molendi 1999; Henriksen et al. 2000; Henriksen & Tittley 2002; Finoguenov et al. 2006; Sanders et al. 2022), or the “Sausage” (CIZA J2242.8+5301; Kocevski et al. 2007; van Weeren et al. 2011; Akamatsu et al. 2015) and “Toothbrush” (1RXS J0603.3+4214; van Weeren et al. 2012; Ogrean et al. 2013; Rajpurohit et al. 2018) clusters showing famous giant radio relics. Instead, candidates for l.o.s. mergers are for instance CL 0024+17 (Czoske et al. 2001, 2002; Ota et al. 2004; Zhang et al. 2005; Jee 2010), Abell 576 (Duck et al. 2007), the “Cheshire Cat” group (Irwin et al. 2015), the Frontier Fields cluster MACS J1149.6+2223 (Ogrean et al. 2016) and complex merging systems similar to Abell 697 from the Reionization Lensing Cluster Survey (RELCIS) (Cibik et al. 2018). Extreme geometrical configurations of cluster mergers can be particularly interesting to pose limits on the detectability of the gas velocity features during and after the dynamical interaction. Furthermore, given the large gas velocities involved, they offer the conditions to test the capabilities of future high-resolution X-ray instruments in reconstructing the ICM velocity field.

Intracluster medium velocities can be in principle measured directly from X-ray observations from the Doppler shift and broadening of emission lines in the ICM X-ray spectrum (see Simionescu et al. 2019, for a recent review). Early direct constraints on ICM bulk motions have been pursued by mapping redshift (i.e., velocity) differences across the system extent, from spatially resolved X-ray observations (e.g., early ASCA measurements on the Centaurus and Perseus clusters by Dupke & Bregman 2001a,b; see also more recent results for Suzaku and Chandra by Tamura et al. 2014; Liu et al. 2015, 2016; Ota & Yoshida 2016). Direct measurements of the ICM nonthermal motions from line broadening are more challenging. In principle, this can be achieved in the case of emission lines from heavy ions, such as the Fe-K complexes at 6.4–6.9 keV. In such cases, the line broadening due to thermal motions is subdominant compared to the broadening and shape distortions caused by bulk and turbulent gas motions. Measurements of these line features requires very high spectral resolution (Inogamov & Sunyaev 2003). Given the typical resolutions of X-ray instruments available, so far most of the ICM velocity measurements actually involved indirect constraints, for instance from measurements of resonant scattering (e.g., Churazov et al. 2004; Sanders & Fabian 2006; Werner et al. 2009; de Plaa et al. 2012; Zhuravleva et al. 2013; Hitomi Collaboration 2018a), or pressure and surface brightness fluctuations (e.g., Schuecker et al. 2004; Churazov et al. 2012; Sanders & Fabian 2012; Gaspari & Churazov 2013; Zhuravleva et al. 2015, 2018). Estimates of ICM motions have also been derived from observations of the SZ (Sunyaev & Zeldovich 1969, 1972; Zeldovich & Sunyaev 1969) effect (e.g., Khatri & Gaspari 2016; Mroczkowski et al. 2019), especially from the kinetic SZ (kSZ, Sunyaev & Zeldovich 1980) signal (e.g., Adam et al. 2017; also explored with simulation studies, Nagai et al. 2003; Baldi et al. 2018). The latter can be particularly strong for merging galaxy clusters, given the large velocities developed (Sayers et al. 2013; Adam et al. 2017). Sayers et al. (2019) employed observations of the kSZ effect toward a sample of 10 merging clusters to constrain the ICM bulk l.o.s. velocity and global RMS gas motions within r2500, which further allowed differentiating between l.o.s. and plane-of-sky mergers. In the X-rays, a few successful attempts were able to place direct constraints on the nonthermal (turbulent) gas velocities in cluster cores by exploiting the Reflection Grating Spectrometer (RGS) aboard XMM-Newton (Sanders et al. 2010, 2011; Bulbul et al. 2012; Sanders & Fabian 2013; Pinto et al. 2015). More recently, an alternative strategy has been presented by Sanders et al. (2020) and Gatsu et al. (2022) exploiting the XMM-Newton EPIC-pn detector. By studying the spatial and temporal variation of fluorescent instrumental background lines present in all observations, they could improve significantly the calibration accuracy and successfully map bulk motions in Coma, Perseus, and Virgo.

So far, the best and only example of direct ICM velocity measurement from high-resolution spectroscopy has been obtained from the observation of the Perseus galaxy cluster by the Hitomi Soft X-ray Spectrometer (SXS) (Hitomi Collaboration 2018b). The high-resolution spectra allowed detailed modeling of the iron He-like Kα complex in the core of the Perseus Cluster, yielding typical ICM bulk velocities and velocity dispersion values on the order of 100–200 km s−1. The unprecedented success obtained with Hitomi confirms the power of high-resolution X-ray spectroscopy, anticipating the further progress that will be achieved with the microcalorimeters on board the next-generation X-ray telescopes, such as XRISM (XRISM Science Team 2020) and Athena (Nandra et al. 2013). These are expected within the next ~15 years, with XRISM launching already by early 2023 and Athena in the early 2030s. Similarly to Hitomi, these will allow for high spectral resolution, namely 7 eV for XRISM Resolve, and 2.5 eV, for Athena X-IFU. If a Lynx-type1 (Gaskin et al. 2019) mission with subarcsecond angular resolution is developed and includes a microcalorimeter, this will provide even further progress, with average spectral resolutions of few eV and arrays optimized to reach fractions of an eV in the soft band. Hydrodynamical simulations are essential to predict the performance of high resolution X-ray calorimeters in the task of mapping ICM velocities, by producing realistic X-ray synthetic observations of simulated clusters (Zuhone et al. 2009, 2016a,b; Biffi et al. 2013; Lau et al. 2017; Roncarelli et al. 2018; Cucchetti et al. 2019; Bulbul et al. 2019).

In this study, we aim to demonstrate, in particular, the capabilities of the XRISM Resolve (Ishisaki et al. 2018) and Athena X-IFU (Barret et al. 2018) to constrain interesting features of the ICM velocity field in extreme merger configurations, via numerical hydrodynamical simulations and synthetic X-ray observations derived from them. Expanding on previous investigations, we also extend our focus beyond the bright central regions of the clusters to fainter regions, such as peripheral locations outside the bright shock fronts formed during the first core passage. We focus on a merging pair of galaxy clusters, with a mass ratio of 1:3 and ICM temperatures of ~5 keV and ~2.5 keV for the main halo and the secondary cluster. This represents a major merger, similar to the case of the “El Gordo” (ACT-CL J0102−4915; Marriage et al. 2011; Menanteau et al. 2012; Zhang et al. 2015; Asencio et al. 2021) but with lower absolute masses of the two components. The structure of the paper is organized as follows. In Sect. 2 we describe the simulations employed and, in Sect. 3, the approach to generate mock X-ray observations of simulated cluster mergers. Results are presented and discussed in Sect. 4, where we investigate the gas velocity field in the merging system after the first core passage, at interesting locations in the

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1 https://wwwastro.msfc.nasa.gov/lynx/; https://www.lynxobservatory.com/
two main projections (perpendicular to the l.o.s. and aligned with it). In this section, we also complement the direct simulation analysis with mock X-ray observations for XRM Resolve and Athena X-IFU. We exploit the larger collecting area and higher spatial resolution of X-IFU to explore also the velocity field across the main shock front. Also, we show predictions for thermal and kinetic SZ effect imaging at the resolutions of CIMB-S4 and the Atacama Large Aperture Submillimeter Telescope (ATLAST; Klaassen et al. 2020). We summarize our results and draw final conclusions in Sect. 5.

2. Numerical simulations

Code. The simulations have been performed with the AREPO code (Springel 2010)\(^2\) and include the treatment of gravity and hydrodynamics only. The AREPO code employs a finite-volume Godunov method on an unstructured moving-mesh to solve the hydrodynamical equations and a Tree-PM solver for solving for the gravitational force.

The simulations we analyze in this work contain three Lagrangian mass elements, that is, gas, DM and stars. The gas elements are simulated using the moving-mesh Voronoi tessellation method. The gas is modeled as an ideal fluid with $\gamma = 5/3$ and mean molecular weight $\mu = 0.6$, that is primordial abundances of H and He with trace amounts of metals. DM and stellar particles only interact via gravity, with each other and with the gas elements. In particular, star particles are included only to serve as tracers of the stellar component associated with the BCG in the cluster center and the average stellar density throughout the cluster. These play no role for the analysis presented in this paper.

For the purpose of the present analysis, no radiative processes such as cooling, star formation or feedback processes are included. For the short timescales and high temperatures involved in the analysis of a merging cluster, these effects are not significant.

The simulations analyzed are noncosmological, that is, the equations of motion have no dependence on redshift. For the purpose of the following calculations and mock observations, we assume a $\Lambda$CDM Universe with $\Omega_{m,0} = 0.27$, $\Omega_{\Lambda,0} = 0.73$ and $H_0 = 71$ km s\(^{-1}\) Mpc\(^{-1}\).

2.1. Merging galaxy clusters

For the current analysis we investigate the properties of a merging system, where two clusters in a 1-to-3 mass ratio collide with zero impact parameter. These are the same initial conditions as in ZuHone (2011), with some changes as outlined here.

The two clusters are initially spherically symmetric and in virial and hydrostatic equilibrium, with parameters consistent with observed relaxed clusters and cluster scaling relations (see Sect. 2.2 of ZuHone 2011 for details). The parameters which we use are given in Table 1.

For the initial total mass distribution of gas, stars, and DM we choose an NFW (Navarro et al. 1997) profile:

$$\rho_{\text{out}}(r) = \frac{\rho_s}{r/r_s(1 + r/r_s)^2}$$

(1)

The scale density $\rho_s$ and scale radius $r_s$ are determined by the virial radius $r_{200c}$ and concentration parameter $c_{200c}$ using:

$$c_{200c} = \frac{r_{200c}}{r_s}$$

(2)

According to the standard definition, $r_{200c}$ corresponds to the radius enclosing an average overdensity of 200 times the critical density of the Universe.

| Cluster | $M_{200}$ [M$_\odot$] | $r_{200}$ [kpc] | $c_{200}$ | $f_g(r_{200})$ |
|---------|------------------------|-----------------|------------|----------------|
| Main    | $6 \times 10^{14}$    | 1639.59         | 4.8        | 0.1056         |
| Subhalo | $2 \times 10^{14}$    | 1136.83         | 5.0        | 0.0879         |

Table 1. Initial cluster parameters.

For the initial total mass distribution of gas, stars, and DM we choose an NFW (Navarro et al. 1997) profile:

$$r_s = \frac{r_{200c}}{c_{200c}}$$

$$\rho_s = \frac{200}{3} \frac{c_{200c}^3}{r_{200c}^3} \rho_{\text{crit}}(2) \left[ \log(1 + r/r_s) - \frac{r/r_s}{1 + r/r_s} \right]^{-1}$$

(2)

where we assume $z = 0.1$ to scale the critical density. The NFW functional form is carried out to $r_{200c}$. Since the NFW mass profile does not converge as $r \rightarrow \infty$, we “taper” the density profile after this radius. For radii $r > r_{200c}$ the mass density follows an exponential profile:

$$\rho_{\text{out}}(r) = \frac{\rho_s}{c_{200c}^3 (1 + c_{200c}^3)^{-1}} \left[ \frac{r}{r_{200c}} \right]^{-\alpha} \exp \left[ -\frac{r}{r_{200c}} \right]$$

(3)

where $\alpha$ is set such that the density and its first derivative are continuous at $r = r_{200c}$ and $\alpha = 1.1$.

The spatial distribution of the stellar mass is divided into two components: a BCG at the cluster center, and a smooth component over the entire cluster representing the stars in the satellite galaxies and the intracluster light. For the BCG component, we use an analytical approximation to a deprojected Sérsic profile given by Merritt et al. (2006):

$$\rho(r) = \rho_s \exp \left[ -d_n \left( \left( \frac{r}{r_{200c}} \right)^{1/n_s} - 1 \right) \right]$$

$$d_n = 3n_s - 1/3 + 0.0079/n_s,$$

(4)

which is a good representation of the stellar mass density profile of elliptical galaxies. We set $n_s = 6$ and use the relationships for BCG masses and radii with their cluster counterparts from Kravtsov et al. (2018) to determine the other parameters for each cluster. We add the contribution to the stellar density from the other galaxies and intracluster light by assuming an NFW profile with the same scale radius as the DM profile and a scale density which is 2% of that of the DM profile.

For the gas, we begin by assuming it has an entropy profile of the form (Voit et al. 2005; Cavagnolo et al. 2008, 2009):

$$S(r) = S_0 + S_1 \left( \frac{r}{0.1 \ r_{200c}} \right)^{\alpha}$$

(5)

where $S_0$ is the core entropy of the cluster and $S_1$ is the entropy at 0.1$r_{200c}$. We initialize our clusters with small core entropies by requiring $S_1/S_0 = 20$, to make our models consistent with relaxed, “cool-core” galaxy clusters, and set $\alpha = 1.1$.

To use this equation to derive the other thermodynamic profiles from the condition of hydrostatic equilibrium, we use the gas mass fraction taken from scaling relations (see Table 1) and impose $T(r_{200c}) = \frac{1}{2} T_{200c}$ (as in Poole et al. 2006), where

$$k_b T_{200c} \equiv \frac{GM_{200c} \mu m_p}{2 r_{200c}}$$

(6)

is the so-called “virial temperature” of the cluster. Once we have the gas density and temperature profiles, we can also derive the dark matter density profile via $\rho_{DM} = \rho_{\text{out}} - \rho_g - \rho_s$. 

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These radial profiles for the gas, DM, and stars can now be used to generate the properties of the particles/cells for the two clusters. To generate positions, we randomly generate a number in the range \(0 < u < 1\) and the function \(u = M_i(r)/M_i(r_{\text{max}})\) is inverted to give the radius of the particle from the center of the halo, where \(i \in [\text{DM}, \ast]\) and \(r_{\text{max}} = 5\) Mpc is the maximum radius of the halo. The gas cell velocities are set to zero in each cluster’s rest frame initially. For the dark matter and stellar particle velocities, we choose to directly calculate the distribution function via the Eddington formula (Eddington 1916):

\[
F(E) = \frac{1}{\sqrt{8\pi^2}} \left[ \int_0^E \frac{d^2\rho}{d\Psi^2} \frac{d\Psi}{\sqrt{E - \Psi}} + \frac{1}{\sqrt{E}} \frac{d\rho}{d\Psi} |_{\Psi = 0} \right],
\]

where \(\Psi = -\Phi\) is the relative potential and \(E = \Psi - \frac{1}{2}v^2\) is the relative energy of the particle. We tabulate the function \(F\) in intervals of \(E\) and interpolate to solve for the distribution function at a given energy. Particle speeds are chosen from this distribution function using the acceptance-rejection method. Once particle radii and speeds are determined, the particle velocities are determined by choosing random unit vectors in \(\mathbb{R}^3\). The masses of the simulated resolution elements are: \(M_{\text{gas}} = 9.22 \times 10^6 M_\odot\), \(M_{\text{DM}} = 6.77 \times 10^7 M_\odot\), and \(M_{\text{star}} = 6.91 \times 10^7 M_\odot\).

The two clusters in the merging system have a virial mass ratio \(M_{200,c,1}/M_{200,c,2} = 3\), with \(M_{200,c,1} = 6 \times 10^{14} M_\odot\) for the main cluster and \(M_{200,c,2} = 2 \times 10^{14} M_\odot\) for the smaller infalling subhalo. We set them up within a cubical computational domain of side \(L = 40\) Mpc. The distance between the cluster centers is given by \(d = r_{200,c,1} + r_{200,c,2} \approx 2.8\) Mpc. Vitrivitska et al. (2002) demonstrated from cosmological simulations that the average infall velocity for merging clusters is \(v_{\text{rel}}(r_{200}) = 1.1 V_c\), where \(V_c = \sqrt{GM_{200,c}/r_{200}}\) is the circular velocity at \(r_{200}\) for the primary cluster. This is then the relative velocity of the two clusters at the beginning of the simulation, \(v_{\text{rel}} \approx 1500\) km s\(^{-1}\). Given that the merger is head-on, the resulting velocity is only in the x-direction, and is given for each cluster in the simulation frame by:

\[
v_{\text{x},1} = v_{\text{rel}} \frac{M_{200,c,2}}{M_{200,c,1} + M_{200,c,2}} \quad (8)
\]

\[
v_{\text{x},2} = -v_{\text{rel}} \frac{M_{200,c,1}}{M_{200,c,1} + M_{200,c,2}} \quad (9)
\]

The gas properties for the cells in the two clusters (which have some overlap in their outskirts) are set by summing the densities and pressures from the two profiles interpolated to the cell positions, and by summing the momenta from each cluster as:

\[
\begin{align*}
\rho(r) &= \rho_1(r) + \rho_2(r) \\
P(r) &= P_1(r) + P_2(r) \\
\rho v_x(r) &= \rho_1(r) v_{\text{x},1} + \rho_2(r) v_{\text{x},2},
\end{align*}
\]

where \(r\) is the 3D coordinate of the gas cell.

Our primary goal is to use this merging configuration to explore the features of the gas velocity field across the merging system and the primary shock front caused by the subcluster infalling through the main halo. We therefore choose a snapshot soon after the first core passage, corresponding to 1.6 Gyr since the beginning of the simulation. This allows us to investigate particularly extreme conditions connected to the geometry of the merger and their impact on the gas velocity distribution, shaping the nonthermal profile of gas emission lines in X-ray spectra. Given that no degeneracies to additional baryonic processes nor to complex chemical distributions are present in the nonradiative run considered here, this enables us to directly explore the possibility to reconstruct such imprints from mock X-ray observations simulating high-resolution X-ray microcalorimeters.

2.2. Numerical estimates

Direct estimates of average i.o.s. velocity and velocity dispersion for the gas selected within a given region in the simulation are given by:

\[
\mu_v = \frac{\sum_i w_i (v_{\text{los},i} - \mu_v)}{\sum_i w_i}, \quad \sigma_v = \frac{\sum_i w_i (v_{\text{los},i} - \mu_v)^2}{\sum_i w_i},
\]

where the summation is performed over the gas elements selected, and \(w_i\) is the weighing quantity (e.g., gas mass, emission measure, Bremsstrahlung-like emissivity or Fe-line emissivity) for the \(i\)th gas element. Values estimated according to Eq. (13) are used in the following sections as expectations and compared against the quantities reconstructed from the analysis of the synthetic X-ray spectra. Typically, we report average numerical values weighted by Fe-line emissivity, to compare more directly with estimates reconstructed from the diagnostics of the Fe-K complex in high-resolution mock X-ray spectra. In these computations, the Fe-line emissivity is an ideal estimate, computed for every gas element (given its thermodynamical properties) from the interpolation of emissivity tables, assuming an APEC model with fixed metallicity (\(Z = 0.3 Z_\odot\)), for the [6.5−7.1] keV rest-frame energy band including the 6.7 keV iron complex.

3. Mock X-ray observations

We generate synthetic X-ray observations from the hot gas properties in the simulated clusters via the pyXSIM Python package (ZuHone et al. 2014)\(^4\), which in turn is based on the PHOX algorithm (Biffi et al. 2012, 2013). While referring the interested reader to the aforementioned papers for further details, we briefly recall here the main features of the approach.

We consider every gas element in the simulation as a single-temperature X-ray emitting plasma, for which the spectral emission follows a thermal Bremsstrahlung continuum with emission lines from heavy ions, implemented as an APEC (Smith et al. 2001) model in the X-ray analysis XSPEC package\(^5\) (Arnaud 1996). Given that no stellar evolution nor chemical enrichment models are treated in our simulations, we assume a uniform metallicity for the ICM equal to \(Z = 0.3 Z_\odot\) and adopt the solar reference abundances of Anders & Grevesse (1989). The simulation snapshot is artificially positioned at a fiducial redshift of \(z = 0.057\), for which the angular scale is \(\approx 1.1 \) kpc arcsec\(^{-1}\) for the LCDM cosmological model adopted here. In the initial phase of generating the ideal sets of photons, we assume artificially large values of collecting area and exposure time to allow for a statistically representative Monte Carlo sampling for later realistic exposures. We also include a Galactic foreground absorption component by using the ‘Tuebingen-Boulder ISM absorption model (tbabs, Wilms et al. 2000) and assuming a uniform fiducial Galactic column density of \(N_H = 4 \times 10^{20} \) cm\(^{-2}\). At a second stage, we project the photons along a chosen i.o.s. direction

\(^4\) pyXSIM (http://hea-www.cfa.harvard.edu/~jzuhone/pyxsim/) critically depends on the yt Project (http://yt-project.org, Turk et al. 2011), to link the hydrodynamical simulations to the algorithm for generating the X-ray ideal photons.

\(^5\) https://heasarc.gsfc.nasa.gov/xanadu/xspec/
4. Results

In this section we compare and discuss the features of the ICM velocity field predicted by the simulations and reconstructed from the synthetic X-ray observations therefrom derived. We concentrate on two l.o.s. directions, perpendicular to the plane of the merger (Sect. 4.1) and along the merger axis (Sect. 4.2). We intend to use these limit cases to constrain the merging signatures in the gas velocity field, at particularly interesting locations in the system.

4.1. Merger in the plane of the sky

We first consider the projection aligned with the \( z \) axis of the simulation box, perpendicular to the plane of the merger. In Fig. 1 we show projected maps, along the \( z \) axis, of the gas X-ray flux (0.5–7 keV rest-frame band)\(^8\), spectroscopic-like temperature\(^9\), and Doppler-shift their energies depending on the l.o.s. component of the velocity associated with the emitting gas element. The final event files are produced by convolving the ideal photon lists with the specific characteristics of the XRISM Resolve and Athena X-IFU instruments, accounting for the effective area, detector response, vignetting, and point-spread function (PSF) of the chosen telescope. This step is performed by means of the SOXS\(^6\) and Simulation of X-ray TElescopes\(^7\) (SIXTE, provided by ECAP/Remeis observatory; Dauer et al. 2019) packages, for XRISM and Athena respectively. Specific details of the synthetic observations we perform are given in the following sections, along with the results.

\(^6\) http://hea-www.cfa.harvard.edu/soxs/

\(^7\) https://github.com/thdauser/sixte

\(^8\) The X-ray flux is calculated from the simulation gas elements, assuming an APEC model with fixed metallicity (Z = 0.3 Z\(_\odot\)).

\(^9\) The spectroscopic-like temperature is an estimate of the gas average temperature often used in cluster simulations and defined as \( T_{\text{sl}} \equiv \frac{\int \rho^2 T^a T dV}{\int \rho^2 T dV} \), with \( a = -0.75 \) (Mazzotta et al. 2004).
l.o.s. EM-weighted velocity and velocity dispersion (from topleft to bottom-right, respectively).

In almost all the X-ray maps, the bright, hot shock front, formed by the secondary bullet halo that passed through the main cluster, is apparent. From the velocity dispersion map, an interesting region with large values of $\sigma_v \gtrsim 600 \text{ km s}^{-1}$ develops on the opposite side of the merger, close to the core of the primary cluster. The symmetry of the merger, that occurs in this projection on the plane of the sky, the l.o.s. bulk velocity is instead typically zero (bottom-left panel in Fig. 1), except for a small region in the brightest central part of the system, where a turbulent eddy has developed after the core passage and residual net negative and positive velocities remain.

On the maps, we mark seven square regions, centered on interesting regions of the merging system, in the vicinity of the shock ($z_1, z_2$ and $z_3$), in the highest velocity dispersion region ($z_5$) and in the brightest part of the system ($z_4, z_4a$ and $z_4b$). Each region, 200 kpc per side, approximates in size the 200 kpc FoV of the XRISM Resolve instrument at the fiducial redshift of $z = 0.057$, where the cluster is positioned for the synthetic X-ray observations.

4.1.1. ICM thermo-dynamical structure along l.o.s.

For each region marked in Fig. 1, we investigate the l.o.s. velocity distribution of the gas directly from the simulation and relate it to the gas thermal and emission properties. Results of this analysis are reported in Fig. 2, for the low-luminosity peripheral regions of the merger (i.e., $z_1, z_2, z_3, z_5$), and in Fig. 3, for the brighter parts of the system (i.e., $z_4, z_4a, z_4b$). In the left-hand-side panels of the figures, we show the distributions of the l.o.s. velocity component, computed directly from the gas elements in the simulation and considering different weights – namely gas mass (black histograms), emission measure (EM; orange), Bremsstrahlung-like emissivity (green) and emissivity of the Fe He-like iron at 6.7 keV (blue).

Phase diagrams mapping the gas velocity and temperature distributions along the l.o.s. are shown in the central column. Here, the color coding marks the total expected emissivity of the Fe K-\alpha complex (as in Sect. 2.2) for the gas in each velocity-temperature bin. The Fe K-\alpha line is a complex of multiple lines, the most prominent of which has a rest-frame energy of 6.7 keV. This emission feature is an optimal target to unveil peculiar motions of the emitting plasma due to the low level of thermal broadening expected for the heavy FeXXV ion (e.g., Inogamov & Sunyaev 2003; Rebusco et al. 2008).

Additionally, we constructed an idealized model of the helium-like iron complex by assuming a single Gaussian centered on the rest-frame energy (6.7 keV) of the most prominent line component and we applied the thermal broadening expected for iron at the given plasma temperature. For each selected region, the right-hand-side plots of Fig. 2 show the shape of the toy-model line, convolved with the gas l.o.s. velocity distribution (blue lines). We also apply an ideal energy smoothing assuming a representative energy resolution of 3 eV in the 6–7 keV energy range (red dashed lines), comparable to the expected resolutions of future microcalorimeters (such as those that will be on board XRISM, Athena, or Lynx). We note that this has no significant impact on the global features of the model lines.

The l.o.s. velocity distribution shows the presence and relative contribution of various velocity components along the l.o.s. in each region. For all the regions investigated, the differences between the various emission-weighted distributions and average values are not significant, so that we mainly refer to the Fe-line emissivity case, with the ultimate goal of studying the Fe-line properties as velocity diagnostics from X-ray spectral analysis. On the other hand, some of the interesting features of the intrinsic, mass-weighted, ICM velocity distribution are reported in Fig. 2, for the low-luminosity peripheral region on the opposite side with extremely high velocity dispersion ($z_5, \sigma_v = 700 \text{ km s}^{-1}$).

Similarly to $z_1$, the other regions in Fig. 2, all relatively faint, show very symmetric double-peaked velocity distributions, due to the symmetry of the merger geometry. In the case of $z_2, z_3$ and $z_5$, however, these features are also present in the mass-weighted velocity distribution and reflected in the velocity-convolved Fe-line shape. Thus, for these regions, the velocity distribution cannot be approximated by a single Gaussian, whereas a Gaussian fit can be attempted for $z_1$. In Table 2, we report the numerical estimates of l.o.s. velocity and velocity dispersion computed from Eq. (13) and compare them to the results from the Gaussian fit of the simulated velocity distributions, when available.

The l.o.s. temperature structure of the gas can further impact the ICM X-ray emission and therefore its spectral modeling. The idealized symmetrical origin of the velocity distributions in Fig. 2 (left) is accompanied by a relatively simple thermal structure, shown in the $\beta_{\alpha} = kT$ phase diagrams (central column panels), where the majority of the Fe-line emission in all cases is dominated by a single temperature component. This also contributes to the negligible differences among the various emission-weighted distributions. As we discuss in the following section, the low surface brightness of these regions poses a serious challenge for deriving constraints on gas velocities from X-ray spectra.

The brighter regions $z_4, z_4a$ and $z_4b$, reported in Fig. 3, exhibit a single-peaked gas velocity distribution along the l.o.s. For the $z_4$ and $z_4b$ regions, in particular, the velocity distributions can be reasonably approximated by a single Gaussian curve, despite the complex velocity-temperature structure of the selected gas (central column). The best-fit Gaussian $\sigma_{v, Fe}$ is in fairly good agreement with the velocity dispersion value computed directly from the simulation (Eq. (13); see Table 2). Differently, the left-most $z_4a$ point shows a very narrow velocity distribution, for which the Gaussian approximation presents
large residuals from the distribution wings, which extend to very large velocity values. These extended faint wings are most likely related to the presence of the shock envelope surrounding the brighter central region, which is characterized by larger gas velocities but is too faint to contribute significantly to the region X-ray emission (see the corresponding velocity-temperature diagram in Fig. 3). We find indeed a significant difference between the best-fit Gaussian $\sigma_{v,Fe}$ ($\sim24$ km s$^{-1}$) and the value of the velocity dispersion computed directly from the simulations ($\sim200$ km s$^{-1}$), with the latter capturing the broader and fainter velocity component as well. Similar conclusions can be derived for the bulk l.o.s. velocity estimates (Table 2). The main features of the ICM velocity distribution in the regions in Fig. 3 are captured by the toy-model Fe line.

The possibility to constrain these l.o.s. velocity distributions via high-resolution X-ray spectroscopy will be explored in the...
Table 2. Comparison between direct simulation estimates and spectral best-fit values of velocity shift and dispersion, for the XRISM Resolve mock observations of the seven regions marked in Fig. 1.

| Theoretical estimate | Gaussian fit | XRISM mock – XSPEC fit |
|----------------------|-------------|------------------------|
|                      | µ_{vFe} [km s^{-1}] | σ_{vFe} [km s^{-1}] | µ_{1} [km s^{-1}] | σ_{1} [km s^{-1}] | µ_{2} [km s^{-1}] | σ_{2} [km s^{-1}] | Exp. [Ms] |
| z1                   | -1.7        | 410.3                  | -7.3           | 485.1           | -21.5 ± 200.3     | 580.3 ± 213.6     | 0.5      |
| z2                   | -0.1        | 220.8                  | -             | -              | -                | -              | 0.5      |
| z3cut                | -2.2        | 416.3                  | -             | -              | -                | -              | 0.5      |
| z4a                  | -8.3        | 200.4                  | 7.8           | 23.7           | 6.4 ± 29.8       | 106.9 ± 46.3     | 0.1      |
| z4b                  | -85.4       | 182.5                  | -62.0         | 153.1          | -77.9 ± 32.0     | 189.7 ± 31.2     | 0.1      |
| z4                   | 3.9         | 327.0                  | 20.9          | 288.3          | -3.0 ± 62.5      | 380.6 ± 60.1     | 0.1      |
| z5                   | 3.8         | 779.7                  | -             | -              | -                | -              | 0.5      |

Notes. In the last column we report the exposure time of the mock XRISM observation.

following via synthetic X-ray observations, assuming the characteristics of next-generation X-ray microcalorimeters, such as XRISM Resolve or Athena X-IFU.

4.1.2. XRISM Resolve mock observations

Our SOXS-based model for the XRISM Resolve soft X-ray spectrometer has a FoV of about 2.9′ × 2.9′ (6 × 6 pixels of 30″ each), a Gaussian PSF with a FWHM of 1.3′, and a RMF with 5 eV spectral resolution. The requirement for the effective area is of ≥160(210) cm² at 1(6) keV. In this section, we present results on ICM velocity diagnostics from mock XRISM Resolve observations of the pointings marked in Fig. 1, whose size (200 kpc per side) approximates the XRISM FoV at the fiducial redshift of z = 0.057. In all cases no background component is included. For bright sources, similar to the z4, z4a and z4b regions, the
Fig. 4. XRISM Resolve images (0.5–2 keV band) for the faint pointings shown in Fig. 2: z1, z2, z3 and z5, from top-left to bottom-right. The images refer to a 500 ks exposure observation. The physical size of each pointing is 200 kpc per side (∼3′ at the assumed redshift $z = 0.057$) and the XRISM Resolve PSF is 1.3′. A physical size of 100 kpc is marked for comparison on the z1 image. The z3 image has been derived for an artificially high spatial resolution (adopting an ideal Chandra-like PSF of 0.5′′) and we mark in red the subregion used to extract the spectrum.

Constraints from spectral analysis. The mock XRISM Resolve images for regions z1, z2, z3 and z5 are shown in Fig. 4. As already noticeable from the idealized flux map (top-left panel in Fig. 1), these pointings are located in faint regions of the system and we adopt therefore an exposure of 500 ks. Even so, only z1 has about 200 counts in the 6–7 keV band, whereas the others have much lower number counts (fewer than 30 photons in the case of z2 and z5). This is not sufficient to perform a spectral fit of the Fe-K complex and reliably constrain the velocity broadening, especially given the complex line structures shown in Fig. 2. Also, the emission of z3 is contaminated by the bright core falling in the rightmost part of the FoV, especially since the ∼1′ PSF scatters photons originating from parts of the core which do not even fall on the Resolve FoV.

For this reason, we treat this pointing differently: we generate an ideal mock observation where the PSF is artificially set to an optimally low value (with a FWHM of 0.5′′) and we mask the core area (rightmost pixel column), while we extract the spectrum from the “z3cut” region (marked by the red box, in the lower-left panel of Fig. 4). By adopting the Chandra-like optimal spatial resolution we minimize the contamination (about 25%) due to photons scattered from surrounding regions and especially from the bright core due to the wide XRISM PSF. Instead, by extracting the spectrum from the z3cut subregion and therefore excluding the core emission (which contributes 30–40% of the total photon counts), we specifically sample the region on the shock front. The spectrum obtained in this way has nevertheless only ≈80(160) counts in the 6–7 keV region for the 500 ks (1 Ms) exposure. Since we have found that >200 counts are required to place stringent constraints on the velocity shift and broadening of the Fe-K line, much longer exposures (>1 Ms) would be required.

The challenge of constraining the velocity broadening from the iron Kα complex at ∼6.7 keV for these faint pointings, due to the poor count statistics, is consistent with previous studies. Predictions for ASTRO-H (Hitomi) indicate in fact that higher number of photons, on the order of $10^3$–$10^4$, are required to...
accurately model the iron complex shape with multiple velocity components (e.g., Shang & Oh 2012; ZuHone et al. 2016a). In Table 2 (three rightmost columns) we therefore only report the best-fit results for the $z1$ mock spectrum, which are consistent with the numerical simulation estimates within the uncertainties.

A different picture is given by the bright pointings located on the central axis of the merging system, $z4a$, $z4b$ and $z4$, for which XRISM Resolve images and spectra (along with best-fit models and residuals) are shown in Fig. 5. With 100 ks exposure, we obtain significantly larger number counts in the XRISM Resolve spectra, ranging between $\approx 400$ and $\approx 1000$ photons in the 6–7 keV band around the Fe-K complex. This allows us to fit an APEC model with line broadening (BAPEC) to the line, in the 6–7 keV band, for which best-fit results for velocity shift and broadening are reported in Table 2.

The spectral best-fit values reported in Table 2 are consistent with the numerical estimates computed directly from the simulation, within the 1-$\sigma$ uncertainties. The difference in the velocity shifts, in particular, are limited to a factor of few-to-ten km s$^{-1}$. The only exception is the case of $z4a$, for which the spectral model provides a lower velocity dispersion value compared to the numerical estimate, despite still being consistent within $\sim 2\sigma$. This was also noted for the Gaussian-fit estimate of the velocity broadening, which is consistently much lower, and related to the shape of the velocity distribution for $z4a$ (Fig. 3, upper-left panel), composed by the superposition of a very narrow central
component and fainter broader wings. Since the spectral fit of the iron complex also assumes a Gaussian distribution of the velocities, any discrepancy between the spectral best-fit values and those estimated directly from the simulation indicate that the Gaussian approximation cannot capture correctly the complexity of the velocity distribution and the presence of multiple l.o.s. velocity components.

1000 mock realizations. We note that the spectral best-fit values reported in Table 2, for all the XRISM Resolve pointings, correspond to average values computed over 1000 realizations for each pointing of the mock observations. This is done to minimize the impact of low-number statistics, related to the random sampling of model emission spectra with low number of counts while generating the mock observations. From the analysis of the 1000 synthetic spectra, we then compute the velocity shift and broadening estimates, and their uncertainties, as the median and robust dispersion of the distributions of XSPEC best-fit values. Median and robust dispersion provide reliable estimates against outliers, therefore mitigating the impact of poor spectra for which the fit does not converge.

4.1.3. Athena X-IFU mock observations

In this section we further investigate the possibility to constrain the ICM velocity field through high-resolution X-ray spectroscopy, in regions characterized by low surface brightness. To this scope, we employ the characteristics of the X-IFU spectrometer, planned to be on-board the ESA Athena satellite and designed to grant a much larger collecting area (\(A_{\text{eff}} \sim 15\,000(1600)\,\text{cm}^2\) at (17) keV), while still securing a very fine spectral resolution (\(\sim 2.5\,\text{eV at } E < 7\,\text{keV}\)) and an angular resolution of \(\sim 5''\) (Barret et al. 2018).

We generate X-IFU synthetic observations of the faint regions centered on \(z_1\), \(z_2\), \(z_3\), and \(z_5\), for which the gas velocity field could not be well constrained with XRISM. The location of these pointings and the corresponding areas covered by the X-IFU hexagonal FoV of \(\sim 5''\) (equivalent diameter) are shown in Fig. 6 (cyan hexagons), where the XRISM pointings are also reported for comparison (green thin squares).

We take advantage of the X-IFU large FoV and collecting area and assume here the reasonable exposure of 100 ks. This allows us to obtain a sufficiently large number of photon counts from the ICM and to perform a reliable spectral fit, in the full 0.2–10 keV energy band (with \(\sim 160\,000\), 5000 and 50\,000 ICM counts for \(z_1\), \(z_2\) and \(z_5\), respectively). In the 6–7 keV range surrounding the Fe-K lines, the net number of counts is about five times larger than in the XRISM spectra, reaching \(\sim 1000\) photons for \(z_1\). For \(z_2\) and \(z_5\), however, it is still quite small, namely \(\sim 200\) and about 10 counts, respectively.

Including the soft part of the spectrum and extending the fit to the full band, for the fainter \(z_2\) and \(z_5\) regions it is thus important to evaluate the impact of the total background emission on the ICM modeling. We thus generate background Athena X-IFU spectra, including both the instrumental Non-X-ray background (NXB) and the cosmic X-ray background (CXB) (e.g., Cucchi et al. 2018). We assume the NXB level equal to the expected mission requirement, namely a constant value of \(5 \times 10^{-7}\,\text{cts}\,\text{cm}^{-2}\,\text{s}^{-1}\,\text{keV}^{-1}\) across the X-IFU FoV, to be renormalized for the full detector area. The physical background comprises both the diffuse unresolved CXB and the astrophysical Galactic foreground. This is modeled as the sum of a soft thermal emission model at low energies (<1 keV), associated with the Galactic plane (unabsorbed) and halo (absorbed) hot plasma, and an absorbed power-law component at higher energies, due to the integrated emission of unresolved extragalactic AGNs. The model and parameters, for an extraction area of 1 arcmin\(^2\), are those reported by Lotti et al. (2014) (as in their Table 2, in which the normalization of the extragalactic component reported in their Table 2 assumes that in real observations of diffuse sources with the Athena X-IFU, given its spatial resolution, AGNs can be mostly resolved to up to 80%).

For the \(z_2\) region, given the low gas temperature, the emission from the cluster ICM is in general fainter (lower intrinsic normalization) than the emission from the background. While we can still attempt an overall fit of the entire 0.2–10 keV energy band, it is not possible to aim for a measurement of the l.o.s. velocity dispersion via the spectral analysis of the Fe-K complexes in the 6–7 keV range alone. Similarly, in \(z_5\), the emission in the 6–7 keV range is also dominated by the (instrumental) background, so that a reliable measurement of the line broadening cannot be obtained.

For these reasons, we use the full 0.2–10 keV energy band to fit the \(z_1\), \(z_2\), and \(z_5\) Athena X-IFU spectra, assuming for the ICM a single thermally broadened APEC model (BAPEC in XSPEC), both with and without background. In all the fits, we fix the abundance and Galactic absorption values to those initially adopted to generate the synthetic observations. The 100 ks X-IFU images of \(z_1\), \(z_2\) and \(z_5\) are shown in Fig. 7 (l.h.s. panels). The spectra, with best-fit models (red curves) and residuals, are shown in the right-hand-side panels of the figure, where the ICM and background components are marked in blue and cyan, respectively. Best-fit results on the l.o.s. velocity and velocity dispersion are reported in Table 3, both for the full mock observations (background included) and for the ICM-only ones.

We also re-compute the values of velocity shift and dispersion directly from the simulation for the new regions with X-IFU FoV sizes. Compared to these numerical estimates, all the best-fit values are roughly within the 1- or 2-\(\sigma\) uncertainties, even when the full instrumental and physical background are included in the mock observation. Although the numerical average values from the simulation are weighted by iron emissivity while the
Fig. 7. *Athena* X-IFU 100 ks mock observations of the faint \(z_1\), \(z_2\) and \(z_5\) pointings: full-band images (l.h.s. panels) and spectra (r.h.s. panels). The best-fit models (red curves) are overplotted on the spectra, with separate components marking the background model (cyan) and cluster emission (blue).

Fits are performed over the full 0.2–10 keV band, we expect the comparison to be robust, given that the shapes of the velocity distributions show negligible differences when different emission-like weights are employed (see Fig. 2).

For both \(z_2\) and \(z_5\), we find that the best-fit spectral results differ from the values computed directly from the simulations, even when the spectrum of the ICM alone without background emission is considered. These discrepancies are related to the intrinsic complexity of the thermodynamical and kinematic properties of the gas in these regions. From the inspection of the \(l.o.s\). velocity distribution of the ICM in these regions – not shown here, but already shown in the smaller corresponding XRISM pointings (see Fig. 2) – we note that poor photon statistics compound the difficulties in fitting a one-component model due to the multicomponent velocity structure of the gas. In particular, this is especially the case for the \(z_2\) pointing, where the low number of counts and the complex shape of the 2-component velocity distribution results in a poor constraint on the velocity broadening. To a lesser extent, also in the \(z_5\) region, the velocity-broadened line shape is very complicated and two temperature components challenge the fitting, although the velocity measurement is nevertheless closer to the theoretical value. In neither of these two pointings, however, is the Gaussian approximation expected to be a fair representation of the velocity distribution.
Table 3. Comparison between theoretical values computed directly from the simulations and spectral best-fit values of velocity shift and dispersion, for the X-IFU pointings centered on z1, z2 and z5.

| Theoretical estimate | Athena mock – XSPEC fit |
|----------------------|-------------------------|
|                      | μvFe, Fe 6−7 keV [km s⁻¹] | σvFe, Fe 6−7 keV [km s⁻¹] | μv(6−7 keV) [km s⁻¹] | σv(6−7 keV) [km s⁻¹] | Exp. [Ms] |
| z1                   | 1.9                      | 395.3                        | 37.9 ± 57.8          | 430.3 ± 54.2          | 497.9 ± 67.9 |
| z2                   | 0.3                      | 201.3                        | 65.5 ± 49.2          | 356.0 ± 54.7          | 125.2 ± 91.4 |
| z5                   | 3.6                      | 766.9                        | 120.1 ± 108.1        | 908.3 ± 98.6          | 806.3 ± 105.5 |

Notes. We report the best-fit results for the spectra of the ICM emission only (columns three and four) and for the complete observations including both instrumental and physical background (columns five and six). The exposure time of the mock X-IFU observations is 100 ks for all pointings (last column).

For the z1 pointing, the larger number of photons in the spectrum and the simpler shape of the intrinsic velocity distribution allow for a better reconstruction of the velocity parameters. Line shift and broadening best-fit values extracted from the ICM-only spectra agree within 1−σ with those computed directly from the simulation. When we include the background components in the mocks, the fit provides poorer constraints, with the best-fit velocity dispersion departing further from the simulation value, although still consistent within 2−σ. In this case, the brighter ICM emission also allows us to perform a fit of the Fe-complex spectral range separately, finding μv [6−7 keV] = −61.6 ± 99.6 km s⁻¹ and σvFe [6−7 keV] = 426.5 ± 89.8 km s⁻¹, when both instrumental and physical background are included. This is still roughly consistent with the full-band fit and is actually in better agreement with the simulation values.

4.1.4. Velocity gradient across the shock front

One of the interesting regions of the merging system studied here is the shock front developing after the first core passage of the two haloes. The z3 pointing, marked in Fig. 1, covers this region. Mock observations with XRISM pointed out the difficulty to constrain robustly the complex velocity structure of the gas. Indeed, the gas velocity distribution along the l.o.s. is characterized by two components and a very complex, double-peaked, non-Gaussian shape (see Fig. 2, third row from the top). This region is moreover one of the fainter ones explored and suffers also from the photon contamination from the bright cluster core nearby. We thus generate mock observations with the Athena X-IFU instrument, to take advantage of its much larger collecting area and superior angular resolution, while preserving the high spectral resolution.

The symmetric geometry of this merger and the velocity field of the gas in the shock indicate the presence of a velocity gradient across the front. To measure the gradient, spectra from several few-kpc-wide annuli must be obtained, requiring a sufficiently large number of photons in each annulus to constrain the gas velocity. To this end, we assume an exposure of 1 Ms for the mock observation with the X-IFU. The 1 Ms image for z3 is shown in Fig. 8, with five annuli defined to map the shock front marked in green. The annuli are separated by 20″, roughly corresponding to 20 kpc. We obtain between ∼76 000 and ∼17 000 photons per annulus, in the 0.2−10 keV band. The full band is adopted for the spectral fit due to the much lower number of photons in the 6−7 keV band, dropping below 200 in the fainter annuli.

We fit each spectrum with a BAPEC model. As in previous Sections, we fix the metal abundance and Galactic absorption to the known input parameters and vary temperature, redshift, velocity dispersion and normalization. We concentrate on the emission of the ICM only and do not include the background.

In Fig. 9, we show a zoom-in onto the simulated maps of gas spectroscopic-like temperature and l.o.s. velocity dispersion, centered on the X-IFU z3 region. In the maps we mark the X-IFU hexagonal FoV and the five annuli on the shock front (numbered from the innermost to the outermost one in the bottom panel). The velocity distributions for gas elements in the annuli are very similar to the double-peaked one shown in Fig. 2, with a spread in velocity that increases with distance from the shock edge. As extreme examples, we only show those for the innermost/brightest (top) and outermost/faintest (bottom) annuli in Fig. 10.

We compare best-fit results for temperature and velocity dispersion against the estimates computed directly from the simulation for each annulus (numbered as in Fig. 9, bottom panel). The temperature and velocity gradients are reported in Fig. 11. In the figure, we report different estimates depending on the band adopted to perform the spectral fit or on the weight used to compute gas velocity and temperature from the simulations, as illustrated in the legend. Given the finely spaced annuli considered here, we also compute the average values from the simulations directly from the 2D regions marked in the projected maps (Fig. 9), to account more properly for the projected gas-cell volume contributing to the emission from such thin annuli. We note that the temperature best-fit values (blue data points) reproduce the gradient across the annuli, with a decrease of average temperature in the direction toward the shock edge. Compared to the spectroscopic results, however, the emission-weighted values from the simulations tend to overestimate the annulus temperature in the faintest ones. The mass-weighted temperature estimate, on the contrary, tends to underestimate the spectral value in the brightest annuli (i.e., annuli 0 and 1). This difference is induced by the more prominent emission of the hot gas in these annuli, which therefore dominates the spectral temperature. If we derive the emission-weighted average temperature from the projected maps (orange diamonds and squares), instead of using the gas element distribution directly (red diamonds), the discrepancy is softened. Overall, the best reconstruction is obtained for the map-derived emission-weighted temperature (orange square), for which the spectral best-fit value is consistent within the 1−σ uncertainties, in all annuli.
The velocity broadening is also closely reconstructed by the spectral fit. For the comparison, we consider the average value in the simulation, weighted either by the emissivity in the Fe-complex (red and orange diamonds), or by emission measure (EM, black square), which has proved to fairly trace the Athena-like spectroscopic value (Biffi et al. 2013; Roncarelli et al. 2018). While all of them provide very similar estimates, the best result is obtained by constraining the velocity parameter on the specific 6–7 keV band, comprising the Fe-complex. The stronger discrepancy with respect to the theoretical values is found in the central annuli (ann. 2 and 3), where nevertheless the spectral value is still consistent with the theoretical one within 1- and 2-$\sigma$. When the velocity dispersion is obtained from the fit over the whole 0.2–10 keV band (blue asterisks), the value is typically poorly constrained, with very large uncertainties, although the overall trend is fairly similar\textsuperscript{11}. Given the large uncertainties on the best-fit values for velocity broadening, the modest velocity gradient across the shock (probing a difference of $\sim$200 km s$^{-1}$ from innermost annulus to outermost one) cannot be well constrained and the spectral fit values are rather consistent with a flat trend.

4.2. Merger along the line of sight

Here we explore the extreme case in which the merger axis of the two clusters is aligned with the l.o.s. Clusters in this configuration, or close to it, might appear as roughly regular clusters in the sky and thus represent a critical challenge for the X-ray mass reconstructions based on hydrostatic equilibrium (e.g., the merging system CL 0024+17; Ota et al. 2004). Such systems can also deviate from the expected scaling relations between mass and observable properties, when substantial bulk and turbulent motions in the ICM contribute to the nonthermal pressure support (Biffi et al. 2013).

In such a l.o.s. merger, significant gas motions are expected to be measured, in particular in the bright central regions, where

\textsuperscript{11} We note that the larger 0.2–10 keV band is in both cases used to constrain the best-fit temperature and normalization.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{image1.png}
\caption{1 Ms X-IFU mock observation (full band) of the z3 region. We mark in green the five 20$''$-wide annuli from which we extract the spectra.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{image2.png}
\caption{Simulated maps of the gas spectroscopic-like temperature and velocity dispersion around the z3 pointing. The Athena X-IFU hexagonal FoV ($\sim$5$''$ equivalent diameter, corresponding to $\sim$330 kpc at $z = 0.057$) and the annuli are shown.}
\end{figure}

the measurement of the double velocity component can thus be more easily obtained. With net velocities of thousand(s) of km s$^{-1}$, the line shifts can be very easily measured and the two merging components distinguished.

Figure 12 shows simulated projected maps of the X-ray (0.5–7 keV) flux and the gas velocity and velocity dispersion along the x-axis l.o.s. (from left to right). The two x1 and x2 regions, approximating in size the XRISM Resolve FoV at the fiducial redshift of $z = 0.057$, sample the central brightest region and an offset fainter location, respectively.

The intrinsic velocity and thermal structure of the gas along the l.o.s. in x1 and x2 are reported in Fig. 13 (upper and lower panels, respectively). Similarly to Figs. 2 and 3, we show the l.o.s. velocity distribution (left) of the gas elements, comparing different weights, the Fe-emissivity of the gas in the temperature-velocity space (middle), and the theoretical shape of the toy Fe line convolved with the l.o.s. velocity distribution (right). From the inspection of the theoretical gas distributions, the two merging components are clearly visible and separate in the $x$1 case. As for the fainter $x$2 pointing, the gas velocity presents a broader, albeit not Gaussian, distribution, originating from the...
complex superposition of regions with different motions along the l.o.s.

In both cases, we use XRISM Resolve mock observations to derive spectroscopic constraints on the gas l.o.s. velocity shift and dispersion. The difference in the brightness of the two regions is remarkable – while a 100 ks exposure for the bright central region x1 ensures more than 1500 counts in the 6–7 keV band, 250 ks are necessary to obtain ≥200 ks counts in the same energy range in x2. XRISM Resolve images (in the soft X-ray band 0.5–2 keV) and spectra (zoomed-in onto the 6–7 keV band), with best-fit model and residuals, are shown in Fig. 14. Table 4 reports the quantitative comparison between XRISM best-fit values and average estimates computed from the simulated distributions\(^{12}\), for the velocity shift and dispersion in x1 and x2. In particular, we note that the brightness of x1 allows for a double-BAPEC spectral fit, leading to a very well constrained reconstruction of the two velocity components, compared to a double Gaussian fit of the theoretical l.o.s. velocity distribution. Only the velocity dispersion of the secondary component (σ\(_T\)) is overestimated with respect to the simulation Gaussian-fit result, although still consistent within the 2-σ uncertainty. This indicates that the two Gaussian functions can capture the complex asymmetrical shape of the velocity distribution. Interestingly, the velocity features of the fainter x2 region are well reconstructed from the spectral fit, despite the non-Gaussian shape of the velocity distribution. We expect, nevertheless, that in this fainter region the background emission – not included here – could compromise this reconstruction.

4.3. Insights from the kinetic Sunyaev–Zeldovich effect

For comparison, we include maps of the thermal and kinetic Sunyaev–Zeldovich effect, characterizing the two respectively by the Compton y parameter, \(y = (\sigma_T/m_e c^2) \int n_e k_BT \, d\ell\), and the so-called \(y_{kSZ}\) parameter, \(y_{kSZ} = (\sigma_T/c) \int n_e v \, d\ell\) (e.g., Mroczkowski et al. 2019), ignoring secondary scattering effects proportional to \(e^{-\tau}\) for electron opacity \(\tau = \sigma_T \int n_e \, d\ell\). As noted in the introduction (Sect. 1), the kinetic Sunyaev–Zeldovich effect can provide additional insight into the internal and bulk motions of the ICM. It can also be used in the definition of \(y_{kSZ}\) that the kinetic SZ traces the momentum of the gas along the l.o.s. The thermal and kinetic SZ signals can be further expressed in terms of the effective CMB temperature (see e.g., the review by Mroczkowski et al. 2019). In particular, the change in \(T_{\text{CMB}}\) due to the thermal SZ effect can be computed from the y parameter as \(dT_{\text{SZ}}/T_{\text{CMB}} = f(x) y\), where classically \(f(x) = xe^{x+1}/(e^x - 1) - 4\) and \(x = hv/k_B T_{\text{CMB}}\) is the dimensionless frequency. Similarly, the strength of the kSZ can be computed knowing \(y_{kSZ}\) as \(dT_{\text{kSZ}}/T_{\text{CMB}} = y_{kSZ}\), where we note that classically the kSZ is simply a Doppler shift in the CMB. This feature of the classical kSZ means it cannot be distinguished from temperature fluctuations in the primary CMB, which are on the order few μK for arcminute scales (e.g., Dunkley et al. 2013).

To assess the utility of the kSZ for providing complementary constraints on ICM motions to those from X-ray calorimeters, we show in Figs. 15 and 16 projections of y and \(y_{kSZ}\) at the resolution of our simulations. In the upper panel of Fig. 15, corresponding to the plane-of-sky merger geometry, the shock front, which is fundamentally a pressure discontinuity, is readily apparent. We note that studies such as those in Basu et al. (2016) and Di Mascolo et al. (2019) have explored similar geometries to constrain the properties of shocks using high resolution observations of the tSZ effect. For comparison of the relative strengths of the tSZ and kSZ signals, we note that near 150 GHz, a frequency often chosen for tSZ surveys, \(f(x)\) is nearly unity in amplitude. This implies that in the l.o.s. case, the strength of tSZ is roughly one order of magnitude greater than that of the kSZ, while for the plane of the sky the tSZ is predicted to be two orders of

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\(^{12}\) Also in this magnitude, we perform 1000 realizations of the mock XRISM observations, to robustly derive the spectroscopic estimates.
magnitude greater. For the l.o.s. merger geometry case, the peak kSZ signal $\gamma_{\text{SZ}} \gtrsim 10^{-5}$ implies it would be detectable above the primary CMB. In a future work we will explore the ability to constrain the merger inclination angle.

We then smooth the maps by 90'' wide, representative of current and near future SZ surveys with, for instance, Advanced ACTpol, Simons Observatory, and CMB-S4 (see Henderson et al. 2016; Abazajian et al. 2019; Ade et al. 2019), and by 10'', representative of larger single dish facilities such as AtLAST, the Green Bank Telescope, the Sardinia Radio Telescope, and the Large Millimeter Telescope (see respectively Klaassen et al. 2020; Dicker et al. 2014; Hughes et al. 2020), as shown in Figs. 17 and 18 respectively. For both resolutions, we choose representative redshifts of $z = 0.057$, $z = 0.3$, and $z = 0.87$, corresponding approximately to the redshifts of the famous massive merging systems A3667, the Bullet cluster, and El Gordo.

It can be seen from the Compton-$\gamma$ images and values of the peak signal that 90'' resolution may not present a critical challenge for TSZ measurements of plane-of-sky mergers at low redshift, where the peak in $y$ is suppressed by 9% at $z = 0.057$. However, by $z = 0.3$ the peak features are suppressed by 35%, and by 58% at $z = 0.87$, which may present a severe limitation.

Fig. 12. Projected maps of X-ray flux in the 0.5−7 keV band (left) and EM-weighted l.o.s. velocity (middle) and velocity dispersion (right), for the x-axis projection, that is with the l.o.s. aligned with the merger axis. The projection is performed over 10 Mpc. Overplotted, the two square X-RISM-like pointings ($x_1$ and $x_2$) of 200 kpc per side.

Fig. 13. Same as Fig. 2, but for regions $x_1$ and $x_2$, where the l.o.s. is aligned with the merging axis. Top panels: ($x_1$), one can notice the asymmetric double component distribution of ICM velocities, corresponding to the two cluster cores.

For systems merging along the l.o.s., the suppression of the peak signal is also similar, albeit slightly larger. By contrast, the $\sim 10''$ or better resolution afforded by larger aperture telescopes shows a much smaller suppression of the peak Compton $\gamma$, which never exceeds 11% in all cases explored, leaving the exciting possibility that next generation high-resolution millimeter observatories may be able to measure it above the primary CMB. We note however that these simulations do not include turbulent subgrid physics akin to that in, for example, Bennett & Sijacki (2020), where even 10'' resolution could limit the observational sensitivity to pressure fluctuations on the smallest scales.
Fig. 14. Left: XRISM Resolve images (0.5–2 keV band) for the x1 (top) and x2 (bottom) pointings shown in Fig. 13. The images (color coded with the same scale for comparison) refer to observations of 100 ks and 250 ks exposure, for x1 and x2 respectively. The physical size of each pointing is 200 kpc per side and the XRISM Resolve PSF is 1.3′.

Right: spectrum, best-fit model and residuals in the 6–7 keV band around the Fe-K line complex, for the XRISM Resolve 100 ks and 250 ks mock observations of the x1 and x2 regions (upper and lower panel, respectively).

Table 4. Comparison between theoretical estimates and spectral best-fit values of velocity shift and dispersion, for the x1 and x2 pointings in the x projection.

| Theo. estimate | Gaussian fit | XSPEC fit | Exp. |
|----------------|--------------|-----------|------|
|                | $\mu_{\text{Fe}}$ | $\sigma_{\text{Fe}}$ | $\mu_1$ | $\sigma_1$ | $\mu_2$ | $\sigma_2$ |
| x1             | $-992.3$     | $591.2$   | $-1629.9$ | $251.7$ | $-630.4$ | $85.2$ |
| x2             | $206.2$      | $437.4$   | $231.0$   | $479.4$ | $-\quad$ | $-\quad$ |

$\mu_{\text{Fe}}$ [km s$^{-1}$] $\sigma_{\text{Fe}}$ [km s$^{-1}$] $\mu_1$ [km s$^{-1}$] $\sigma_1$ [km s$^{-1}$] $\mu_2$ [km s$^{-1}$] $\sigma_2$ [km s$^{-1}$] $\mu_1$ [km s$^{-1}$] $\sigma_1$ [km s$^{-1}$] $\mu_2$ [km s$^{-1}$] $\sigma_2$ [km s$^{-1}$] $\mu_1$ [Ms]

For $x1$ only, the Gaussian fit of the simulation velocity distribution and the XSPEC fit are both performed with two Gaussian components, in order to approximate the 2-component velocity distribution shown in Fig. 13 (upper panels).

5. Summary and conclusions

In this work, we explored the possibility to constrain the ICM velocity field in a major cluster merger by means of X-ray microcalorimeter observations, anticipating the expected performance of XRISM Resolve and Athena X-IFU. Especially for complicated structures of the velocity field along the l.o.s. due to extreme geometrical configurations, X-ray spectra with an energy resolution of a few eV from upcoming microcalorimeters will be essential. We analyze the three-dimensional thermal and velocity structure of the ICM in a hydrodynamical simulation of a major merger between two clusters, with zero impact parameter and a mass ratio of 1:3. We focus on a snapshot in time soon after the first core passage. We also
provide predictions on the SZ view of these same merger geometries.

Our main findings can be summarized as follows:

- From the direct inspection of the simulated system we find significant nonthermal velocity dispersion at various locations, reaching several hundreds km s\(^{-1}\), both in the projection perpendicular to the merger direction and along the l.o.s. aligned with it.

- By inspecting the simulated l.o.s. velocity distribution, we notice that large velocity dispersion values can often be ascribed to multiple velocity components with large velocity differences, in line with observational constraints from redshift mapping of merging clusters (see Liu et al. 2016). Thus, the detailed line shape is expected to be manifestly non-Gaussian in such cases.

- While substantial net I.o.s. velocities on the order of \(\sim 1000\) km s\(^{-1}\) develop when the merger direction is aligned with the I.o.s., the plane-of-sky merger shows negligible shifts of the emission line centers, corresponding to no net bulk I.o.s. motions (Sayers et al. 2019). This is consistent with estimates for the Bullet Cluster obtained by Liu et al. (2015). We have shown that negligible values of the net I.o.s. velocities, can be due to a symmetrical, albeit broadened, distribution of the I.o.s. gas velocities or to a multicomponent distribution with roughly opposite line shifts, which nevertheless does not imply an intrinsically low level of nonthermal or bulk motions. This finding suggests caution in reconstructing gas motions from the Doppler shift of emission lines, which can misleadingly under-estimate the amount of nonthermal motion in plane-of-sky merging systems.

- XRISM Resolve observations of bright regions can successfully constrain the velocity dispersion from the iron Kα complexes in the 6–7 keV band with 100 ks exposures. Some discrepancy with respect to the expected value derived from the direct simulation analysis can be ascribed to the non-Gaussian shape of the iron line, due to the complexity of the velocity distribution along the I.o.s. For the I.o.s. merger, the two components associated with the two system cores can be reconstructed (both shift and broadening) from the double-component spectral fitting of the 6–7 keV band, assuming a typical 100 ks observation of the central bright region.

- The velocity broadening in fainter regions, e.g., beyond the shock edge of the plane-of-sky merger, cannot be successfully constrained from XRISM spectra, despite the large values, due to poor photon statistics.

- The larger effective area of Athena X-IFU allows for consistent estimates of ICM velocities compared to the simulation values in relatively faint regions. This result is obtained using a reasonable 100 ks exposure, and accounting for instrumental and physical background as well. A detailed reconstruction of the two symmetrical velocity components by means
of the superposition of two Gaussian terms was not possible, due to the poor photon statistics.

A velocity dispersion gradient downstream of the shock is developed in the plane-of-sky projection of the merger. By analyzing *Athena* X-IFU spectra extracted from five 20''-wide annuli across the shock, we reconstruct temperature and velocity dispersion values that are roughly consistent with the estimates computed directly from the gas-cell distributions. While the temperature gradient is indeed recovered, the moderate velocity dispersion gradient cannot be well constrained, given the large uncertainties on the best-fit values of velocity broadening. The expected velocity dispersion values are indeed relatively low, decreasing from ~400 km s\(^{-1}\) to ~200 km s\(^{-1}\) from the innermost annulus to outermost one.

Fig. 17. Noise free, smoothed thermal SZ images of the plane-of-sky (upper six panels) and line-of-sight geometries (lower six panels), corresponding to the upper and lower panels of Fig. 15. First and third rows: images for an AtLAST-like resolution at 150 GHz, second and third rows: images for a CMB-S4-like resolution. The columns correspond to the representative redshifts of \(z = \{0.057, 0.3, 0.87\}\), chosen to correspond, for example, to the mergers in A3667, the Bullet Cluster, and El Gordo.
From the inspection of the expected SZ thermal and kinetic signals derived for the resolution and redshift \( z = 0.057 \) of our simulation, we find that the strength of tSZ is one and two orders of magnitude greater than the strength of kSZ, in the l.o.s. case and plane-of-sky merger respectively.

By assuming typical resolutions of current surveys (90') and large single dish facilities (10'') at low, intermediate and high redshifts, we note that the suppression of thermal SZ signal is not as severe as in the case of kSZ, especially at high resolution. For plane-of-sky mergers at low redshifts, measurements of the thermal SZ can provide informative constraints also at low resolution. More severe limitations are expected in the case of the kSZ signal, for which high resolution facilities such as AtLAST are definitely required to constrain the
ICM velocity features even in the case of mergers aligned along the l.o.s. We have shown that ICM motions, developing after a major merging event, can be in many cases well constrained with X-ray microcalorimeter observations. While XRISM can be safely employed in bright cluster regions, fainter ones—e.g., merging event, can be in many cases well constrained with the Athena X-IFU, or exposure times larger than 1 Ms.

The cases discussed in this work present some similarities with well-known observed systems, such as the disturbed clusters Abell 754 or Abell 3667. In these cases, the shock front, in the plane-of-sky merger configuration, constitutes a real challenge to constrain gas motions in the shock region with XRISM Resolve (consistent with predictions in Kitayama et al. 2014), especially for the moderate turbulent velocities expected there ($\lesssim 300$ km s$^{-1}$, from our simulation). Longer XRISM exposures on fainter off-set regions can only provide realistic constraints when the turbulent broadening is larger (e.g., on the order of $400-500$ km s$^{-1}$, for our $z_1$ pointing). Microcalorimeters similar to Athena X-IFU, with a larger effective area and smaller PSF, will greatly improve the reconstruction of both streaming and turbulent motions in fainter regions.

The most challenging aspect still remains the detailed reconstruction of the line shape, which is nevertheless crucial to distinguish between true turbulent broadening and superposition of l.o.s. streaming motions. ZuHone et al. (2016a), focusing on XRISM-like mock observations of bright central cluster regions in a relatively relaxed cluster with sloshing motions, also found that large number counts ($10^3$ or more) in the iron complex band are required to fully model the multicomponent line shape. This is consistent with expectations obtained for observed systems in the preparatory studies for ASTRO-H Kitayama et al. (2014).

Even for the Athena X-IFU, Roncarelli et al. (2018) showed that very large exposures, on the order of several Ms, would be required to fully reconstruct the velocity structure function and velocity field, and to account for a full thermodynamical description of the ICM. Zhuravleva et al. (2013) constructed model spectra, assuming a large number of photons, to provide templates for the expected distortions of emission lines due to resonant scattering. In their theoretical study, they predicted the possibility to constrain such signatures with 100 ks ASTRO-H (XRISM-like) observations of the Perseus cluster core, considering a Gaussian shape of the lines (see also predictions from ZuHone et al. 2016b). Cucchi et al. (2019) also investigated the possibility to statistically map the ICM velocity field through studies of the structure function from simulated Athena X-IFU observations with typical exposures of 100 ks. They also extracted the spectra from binned regions to reach high signal to noise ratios (with $\sim 40,000$ counts).

Despite the idealized set-up of our simulated merger, we showed that the low number counts in the iron 6–7 keV band, combined with a complex thermal gas structure along the l.o.s., can prevent a detailed reconstruction of complicated line shapes, for moderate exposures. A successful multi-Gaussian modeling, similarly to that proposed by Shang & Oh (2012), requires very large photon counts ($\geq 1000$ in the Fe-K band). As we discussed, this can be definitely achieved with a single 100 ks Athena X-IFU observation for the bright central region of a l.o.s. merger (see Sect. 4.2), where the multiple velocity structures can be well constrained.

The possibility to combine observations with X-ray calorimeters and SZ data can further provide valuable insights on the ICM velocity field in merging systems. Current and upcom-

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