Identifying dark matter haloes by the caustic boundary

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Abstract. The dark matter density is formally infinite at the location of caustic surfaces, where dark matter sheet folds in phase space. The caustics are boundaries between the regions with different number of streams $n_{\text{str}}(x)$ in Eulerian space. Alternatively they can be defined as boundaries between the regions with different number of flip-flops $n_{\text{ff}}(q)$ in Lagrangian space. The number of flip-flops equals the amount of turns inside out experienced by a fluid element of a collision-less medium. Physically both definitions are equivalent but discreteness of numerical models may result in some distinctions. After $n_{\text{str}}(x)$ or $n_{\text{ff}}(q)$ field is numerically evaluated the identification of caustics becomes a purely geometrical procedure which is independent on any numerical parameters. Both approaches are used in identifying a compact closed caustic surface around potential halos in an idealized N-body simulation. The set of all caustics should be the same in both cases, but comparing $n_{\text{str}}(x)$ and $n_{\text{ff}}(q)$ is not straightforward because there is no simple relation between the number of streams and number of flip-flops. The halo boundary in this simulation is found to be neither spherical nor ellipsoidal nor oval but remarkably asymmetrical. However, a convex hull is a good approximation to the halo boundaries. The analysis of the kinetic and potential energies of individual particles and the halo as a whole concludes that it is gravitationally bound. In addition, the examination of the two-dimensional phase space confirms the above conclusion. The recent finding that common shells in a sample of halos obtained from the suite of large simulations are non-ellipsoidal ovals is quite encouraging for carrying out a more detailed analysis of this approach on higher resolution simulations.

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Caustics along with the multi-stream regions and flip-flop field are inherent features of the cold collision-less dark matter (DM) web. Known in geometric optics as an envelope of light rays reflected or refracted by a smooth curved surface a caustic is a line or point where the light intensity approaches infinity when the wavelength of the illuminating light tends to zero. The Zeldovich Approximation (ZA) [1] in two-dimensional space is identical to refraction of parallel light rays by a plate with thickness given by a two-dimensional random smooth function. When a screen is placed behind the plate then bright caustic patterns can be observed in a certain range of distances from the plate. These patterns are exactly the same as the web structures predicted by the ZA in two dimensions [2, 3]. The intensity of light in caustics is high but finite since the wave nature of light. Similarly the density in
caustics in a cold collision-less DM is high but finite because of two reasons. First, DM is not a continuous medium, second — more importantly — DM has a very small but finite velocity dispersion. However, the smaller the velocity dispersion the higher density in the caustics, see e.g. [4]. Anyway the approximation of DM by a cold continuous medium is extremely accurate and commonly used in cosmology.

The DM web possesses two additional traits that cannot be found in a collisional medium like baryonic component in the universe. They are multi-stream flows and flip-flops of fluid particles. All three are closely connected but not identical phenomena. A flip-flop field is the count of turns inside out for each fluid element. Flip-flops are similar to caustic counts introduced and used by [5–8]. Both become the same quantity in the continuum limit but differ simply in their numerical inference of it. They can be used as additional quantitative characteristics of the DM web. The multi-stream field is simply a count of the streams with distinct velocities at every point in Eulerian space. Generally the number of streams is an odd integer except the caustic surfaces where it is an even integer.

Both can be evaluated in cosmological N-body simulations. It can be done either on particles or tetrahedra in the tessellation of the three-dimensional phase space sheet in six-dimensional phase space [9, 10]. The tessellation technique allows to considerably improve N-body simulations [11–13] and provides additional effective diagnostics for the analysis of the complexity of the DM web [14–18].

An idea that the formation of a halo in generic case requires three collapses along three orthogonal axes corresponding to three eigen values of the deformation tensor was suggested in the frame of the ZA [19]. A region where the fluid elements have experienced collapses along three, two or one eigen vector is classified as halo, filament or pancake/wall respectively. The fluid elements that have experienced no collapses and are beyond multi-stream regions belong to voids. A physically similar proposition was recently reintroduced in two different mathematical and numerical forms. One of them known as Origami method assigns morphologies (void, wall, filament or halo) of particles based on the number of orthogonal directions along which the Lagrangian origami manifold is folded: 0, 1, 2, or 3 respectively [20]. The other is based on the analysis of the evolution of an infinitesimal Lagrangian fluid element traced by the Geodesic Deviation Equation [5–8].

The multi-stream field in N-body simulations is naturally to evaluate on arbitrary set of diagnostic points in Eulerian space [15, 21, 22]. On the other hand the flip-flop field can be easily computed on particles or tetrahedra [14, 18]. In Lagrangian space it is a field i.e. a single valued function. Mapped to Eulerian space it becomes a multi-valued function which is more difficult to deal with. Caustics border the regions with different values of flip-flops in Lagrangian space or between regions with different number of streams in Eulerian space.

In principle caustics surfaces can be identified as very thin layers of very high DM densities but it would require N-body simulations with unfeasibly high mass resolution for current N-bogy techniques. However, since caustics separate the Lagrangian neighbor elements with different number of flip-flops it is also possible to use the common faces of two neighboring tetrahedra with opposite parities as an approximate representation of the elements of caustic surfaces [9, 10].

Topological analysis and classification of all generic types of caustics originating in a potential mapping of a collision-less medium in two and three dimensions were provided in [23]. However, the analysis was based on the so called normal forms which roughly speaking are the minimal polynomials used as generators of singularities. In this form the results can be used only as a solid guideline for the much more strenuous analysis of realistic DM
flows in cosmological simulations. The first analysis of the geometry and topology of the caustic structures in the frame of the ZA with smooth random initial perturbations was done in [24], however, it was limited to two dimensions. For the recent scrutiny of the subject see [25] and [26].

The presence of caustics has been implied in many cosmological N-body simulations. For example, a splashback radius defined as the distance from the center of a halo to its outermost closed caustic in the spherical models as an alternative to virial radius for defining boundaries of DM haloes [27, 28]. The authors argued that the splashback radius is a more physical choice of the halo’s boundary than one based on a density contrast $\Delta$ relative to a reference density (mean or critical). However, they did not identify caustics directly. Instead they searched for a minimum of the logarithmic slope of the spherically averaged density profiles of the haloes. Spherical averaging of the density profiles may enhance the robustness of the results but it imposes an assumption that haloes can be well described as spherical configurations.

The studies of caustics are often conducted in the context of indirect detecting of dark matter, e.g. [29, 30]. However, the caustics are the surfaces where the DM flows experience extraordinary metamorphoses. The tessellation tetrahedron turns inside out when one of its vertices crosses the face of the tetrahedron defined by the remaining three vertices. Caustics provide natural boundaries between different states of a collision-less medium represented by the number of flip-flops. The focus of this paper is on constructing caustics as triangulated surfaces with the vertices on particles of N-body simulations. The major difficulty is a sampling problem which is of course not a new one. It has been long known that sampling along with the mass and force resolutions plays a crucial role in delineating the internal geometry of the filaments and walls. The importance of having a sufficiently high density of mass tracers for disclosing the structures was demonstrated in 2D N-body simulations [31, 32]. In particular, the structures obtained in the simulations with physically identical initial conditions but with different number of mass tracers were compared. A plot with $256^2$ particles demonstrated complicated internal structures arising at late nonlinear stages. However, exactly same structures were practically invisible rendered with $64^2$ particles. Here is a recent example of stressing the mass resolution. It was demonstrated that in order to reliably trace the evolution of subhaloes in a strong tidal field each subhalo must have at least 1000 particles [33]. The simplest way to overcome this problem is to apply the approach of [31, 32] to three-dimensional case, i.e. to run an idealized N-body simulation which is described in section 3.

In section 2, we briefly discuss caustic formation in the context of the Zeldovich approximation. We explain our choice of the parameters in our N-body simulation in section 3. Section 4 describes the details of our algorithm using the Lagrangian tessellation scheme. In section 5, we carry out the analyses of the caustic surfaces and their relation to multi-stream field. Section 6 describes the dumbbell structure and discuss the velocity field within it. Two convex hull approximations using either the number of flip-flops on particles or the vertices of caustic triangles are compared in section 7. Finally we summarize the results in section 8.

2 Theory of caustics and streams

2.1 Caustics in the example of the Zeldovich approximation

In this section we introduce the concept of singularities in a cold continuous collision-less medium. All three requirements are necessary and sufficient for the formation of singularities
in the density field. Cold dark matter (CDM) is an almost perfect example of such a medium. We begin with a brief illustration by describing the evolution of CDM density field according to the Zeldovich approximation. The ZA is an elegant analytical approximation to describe the early phase of the non-linear stage of the growth of density perturbations. Technically it is a first order Lagrangian perturbation theory known as LPT1. However, Zeldovich suggested to extrapolate it to the beginning of the non-perturbative nonlinear stage and predicted the formation of caustics which are the boundaries of the very thin multistream regions dubbed by him as ‘pancakes’. The ZA describes a dynamical mapping from the initial Lagrangian space with coordinates \( q \) to Eulerian space \( x(t) \) at time \( t \). In comoving coordinates, \( x = r/a(t) \) where \( a(t) \) is the scale factor normalized by \( a(z = 0) = 1 \) and \( r \) are the physical coordinates of particles at time \( t \) the ZA takes the form

\[
x(q, t) = q + S(q, t) = q + D(t) s(q),
\]

where \( D(t) \) is the linear density growth factor. The potential vector field \( s(q) = -\nabla_q \psi(q) \) is determined by the potential \( \psi(q) \) which is proportional to the gravitational potential at the linear stage. Conservation of mass implies \( \rho(x, t) d^3x = \rho_0 d^3q \), so the density field in terms of Lagrangian coordinates is given at \( t > 0 \) as

\[
\rho(q, t) = \rho_0 \left| J \left[ \frac{\partial x}{\partial q} \right] \right|^{-1},
\]

where the Jacobian \( J \left[ \frac{\partial x}{\partial q} \right] \) is calculated by differentiation of Equation 2.1. Moreover, diagonalization of the symmetric deformation tensor \( d_{ij} = -\nabla_q s(q) = \partial^2 \psi(q)/\partial q_i \partial q_j \) in terms of its eigenvalues \( \lambda_1(q), \lambda_2(q), \lambda_3(q) \) particularizes the patterns of collapsing of the fluid elements. This reduces the equation describing the mass density to a convenient form

\[
\rho(q, t) = \frac{\rho_0}{\left| 1 - D(t) \lambda_1(q) \right| \left| 1 - D(t) \lambda_2(q) \right| \left| 1 - D(t) \lambda_3(q) \right|}.
\]

Since the deformation tensor \( d_{ij} \) (known also as deformation gradient tensor or distortion tensor) and its eigenvalues depend only on the initial fields, the ordered eigenvalues defined in Lagrangian space \( \lambda_1(q) > \lambda_2(q) > \lambda_3(q) \) determine collapse condition for fluid elements in Eulerian space. With the growth of \( D \) with time, the mass density of cold continuous fluid can rise until reaching singularity at \( D(t) = 1/\lambda_1(q) \).

Locally in Lagrangian space, the condition \( \lambda_1(q) = 1/D(t) \) firstly takes place at a maximum of \( \lambda_1(q) = \max = 1/D(t_b) \) where \( t_b \) denotes the time of the ‘pancake’s birth’. At later times \( t > t_b \) the caustics are the level surfaces of constant value of \( \lambda_1(q) = 1/D(t) < 1/D(t_b) \) mapped to Eulerian space by Equation 2.1. At small \( \delta t = t - t_b \) the level surfaces are closed and convex in Lagrangian space. In Eulerian space at time \( t \) they form the surfaces where density becomes formally infinite — therefore the term a caustic.

At a randomly chosen point \( q \) three eigenvalues are always distinct from each other if the perturbation potential \( \psi(q) \) is a generic field. Three fields \( \lambda_1(q), \lambda_2(q) \) and \( \lambda_3(q) \) are non-Gaussian even when \( \psi(q) \) is a Gaussian field. In the case of the Gaussian potential the joint PDF of three eigenvalues can be found in analytic form (see e.g. [34, 35]). It contains a factor \( (\lambda_1 - \lambda_2)(\lambda_1 - \lambda_3)(\lambda_2 - \lambda_3) \) which explicitly shows that the chance of finding a point with two or three equal eigenvalues is negligible.

For more detailed analysis of the geometry and topology of the caustic structures in two-dimensional case we refer to [24] and [25]. Unfortunately a detailed analytical characterization
of three-dimensional ZA with generic initial perturbations has not reached a comparable level yet. However, an important step forward has been recently made in [26].

### 2.2 Caustics and streams in previous N-body studies

The collapse of a region where all three eigen values are positive proceeds as a sequence of three collapses along three mutually orthogonal directions determined by three eigen vectors: $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$. But of course, the ZA breaks very quickly after the first collapse especially along $\mathbf{e}_1$ that corresponds to $\lambda_1$. However, the collapses along $\mathbf{e}_2$ and later along $\mathbf{e}_3$ keep going even the actual collapse along $\mathbf{e}_1$ becomes very different from one predicted by the ZA. As a result one may expect that halos may originate from the peaks of smallest eigen value field $\lambda_3(q)$ in Lagrangian space. An N-body simulation in the hot dark matter cosmology showed that this prediction based on the ZA is generally correct [19]. The conclusion of that study stated that the formation of a halo requires at least three collapses along three orthogonal axes: first to a pancake, second to a filament, and only after that to a halo. They are determined by three conditions imposed on the eigenvalues: $\lambda_1 > 0$, $\lambda_2 > 0$, and $\lambda_3 > 0$ respectively. However, this represents a fundamental limitation of the ZA.

A physically similar idea was suggested in the ORIGAMI model [20]. The halo particles are identified as those that have undergone shell-crossing along three orthogonal axes. The other types of the large-scale structure are associated with the particles that have undergone two, one or zero shell-crossing along orthogonal axes that correspond to filaments, walls/pancakes, and voids, respectively. A more general approach based on the distortion tensor $D_{xq}$ maps a unit sphere in Lagrangian space to a distorted ellipsoid in Eulerian space [7] has come to a qualitatively similar conclusions [8]. It is remarkable that three technically very different approaches agree at least qualitatively.

The geometrical and topological complexities of the caustic surfaces in three-dimensional configuration space are due to the maze-like map of the three-dimensional hypersurface $x(q)$ called the Lagrangian submanifold from six-dimensional ($q, x$)-space into three-dimensional $x$ space [9, 10]. The Lagrangian submanifold is a single valued, smooth and differentiable vector function $x = x(q)$. But its projection into three-dimensional Eulerian space creates creases, kinks and folds. Note that $x(q)$ and $v(x)$ submanifolds are very different, though, they are connected by a canonical transformation. Delineating the Lagrangian submanifold reveals several properties of the dark matter dynamics not inferred from position-space analyses. Two physically related fields — the multistream field $n_{str}(x)$ in Eulerian space [9, 15–17, 21] and the flip-flop field $n_{ff}(q)$ in Lagrangian space [8, 14, 18] are instrumental for the analysis of the Lagrangian submanifold.

The number of flip-flops explicitly evaluated in cosmological N-body simulations currently does not exceed a few thousand [7, 18]. The directly registered number of streams does not exceed $\sim 10^5$ [10]. The number of streams, as estimated from the fine-grained stream densities of individual simulation particles, suggest that at a typical point at 8 kpc from the halo center of DM Milky Way haloes simulated in the Aquarius Project about $10^{14}$ streams [7]. The number of flip-flops is always less than the number of streams. For instance, consider the one-dimensional collapse of a sinusoidal density perturbations. The fluid elements of the central part of the halo experience the greatest number of flip-flops at all times. If the maximum of flip-flops is $n_{ff,\text{max}}$ then the maximum of the number of streams becomes $n_{str,\text{max}} = 2n_{ff,\text{max}} + 1$. In addition, the process of merging of haloes may considerably increase the number of streams without significant effect on flip-flop counts. Unfortunately, there is no simple relation between numbers of flip-flops and streams in a general case.
3 N-body simulation

We carried out our simulations with the ‘standard’ ΛCDM cosmology, Ω_m = 0.3, Ω_Λ = 0.7, Ω_b = 0, σ_8 = 0.9, h = 0.7. In order to compute flip-flops we used a slightly modified version (for details see [18]) of a publicly available cosmological TreePM/SPH code GADGET [36].

In order to create a sufficient particle sampling we introduce an artificial spherically symmetric sharp cutoff in the initial spectrum of perturbations — a standard option in GADGET. Our simulations differed from each other by four parameters: number of particles N_p^3, the size of the box L and the force softening scale R_s both in units of Mpc/h, and a cutoff scale k_c defined in GADGET by the parameter n_c according to equation k_c = (2π/L)(N/n_c). In other words it means that the initial power spectrum P(k) = 0 for all k > k_c.

After trying a number of different sets of the parameters we have selected one that fits our major goals. The size of the box is L = 100 Mpc/h, the number of particles N_p = 256^3, the force softening scale R_s = 0.78 Mpc/h, and the cutoff scale parameter n_c = 64 which means that the initial spectrum covers a very small range from k_min = (2π/L) to k_max = k_c = 4k_min. The choice of R_s about two times greater than a mean particle separation l_0 ≈ L/N_p = 0.39 Mpc/h has been made in order to preserve the phase space sheet from self-crossing for longer period of time. As it was demonstrated in the one-dimensional oblique plane wave collapse test the discrepancy between the 3D N-body solution and the true one-dimensional solution already exists at shell-crossing and becomes more severe at later times already at R_s = 0.5l_0 [37]. Later this result was confirmed and elaborated by additional more sophisticated tests in [11, 13, 38]. Increasing R_s in our simulations to R_s ≈ 2l_0 significantly relieves the problem of the self-crossing of the phase space sheet. The initial power spectrum of this idealized simulation is similar to that in HDM simulations in 100h^{-1}Mpc box by [39]. The major difference is at k ≳ 0.1h Mpc^{-1}: in our simulation P(k) = 0 while in the HDM model P(k) falls exponentially so that P(k) drops off almost seven times at k = 0.2h Mpc^{-1}. The other difference is in the force softening length: it was about twenty times less than in our simulation.

The cutoff in the initial power spectrum requires slightly more than a hundred random numbers for the generation of initial perturbations. The number is obviously far too small for any statistical valuation but it is more than sufficient to guarantee the initial conditions to be of a generic type. Specifically it means that if this type of initial conditions is used in the ZA then all and only singularities which are listed in [23, 24] can emerge in the non-linear regime. The displacement vector field S(q, t) = x(q, t) − q acquires a solenoidal component in the non-linear regime. This is an additional source of inaccuracy in the ZA. However, this happens regardless of the length of the initial power spectrum. Of course, the complexity of the nonlinear structure will increase with the growth of the initial power spectrum at least at some stages.

Our idealized model allows a reliable identification of several generations of internal caustics. We also were able to simulate one of the most fundamental structures in DM web. It is a dumbbell structure consisting of two haloes connected by a cylindrical filament. As we mentioned in section 1 numerous images of this structure are shown in figure 1 in [40]. However, due to a small range of the initial power spectrum this simulation can be regarded only as the first successful attempt to directly build the caustic surfaces in cosmological N-body simulation started from a very smooth random field. Our choice of the cutoff scale approximately corresponds to the scale of clusters of galaxies. It may very roughly illustrate
the formation of clusters of galaxies in the HDM scenario and perhaps first haloes in WDM and CDM models. Figure 1 provides a sense of the evolution of the structure in the simulation at the nonlinear stage. It shows the monotonic growth of the number of particles experienced flip-flops and the decrease of the number of particles with zero flip-flops $N_p(n_{ff}, a)$. It is also worth noting an orderly behavior of $N_p(n_{ff}, a)$: $N_p(n_{ff}, a) > N_p(n_{ff} + 1, a)$ for all $a$ and $N_p(n_{ff}, a_2) > N_p(n_{ff}, a_1)$ for all $n_{ff}$ if $a_2 > a_1$. The number of particles drops from $\approx 10^6$ at $n_{ff} = 1$ to $\approx 10^4$ at $n_{ff} = 6$. It is worth stressing that the number of vertices in the caustics in the region we discuss in section 5 is 10–100 times less as table A in appendix A indicates.

It is worth mentioning that the statistics presented in figure 1 depends on the initial power spectrum. In particular, if small scale power is kept down to scale 0.01 Mpc/h or less almost all of the mass is going through 1 or more flip-flops [22].

\section{Identification of caustics in numerical simulations}

Finding caustics in numerical simulations by the ZA as well as by N-body techniques could be made by various methods. One can do this by analyzing singularities of the eigenvalue fields of the deformation tensor $\partial s_i / \partial q_j$, where $s_i(q, t) = x_i(q, t) - q_i$. In the case of the ZA it is simply $D(t)s_i(q)$ in Equation 2.1. In the case of N-body simulations it requires numerical calculation of the positions of the particles at time $t$. The passage of a particle through the singular stage corresponds exactly to the sign change of the Jacobian $J$ (Equation 2.2), see e.g. [7, 18]. This method allows to count how many times a particle has passed through the caustic state which is equivalent to the number of flip-flops computed for each particles. The probe of the geometry and topology of caustics requires to analyze the spacial structure of the eigenvalue fields [24–26].
In this paper we will use a different method of finding caustic surfaces directly from the Lagrangian triangulation [9, 10]. First we need to evaluate the volume of every tetrahedron in the tessellation. It can be done by computing the following determinant for each tetrahedron

\begin{equation}
    d = \begin{vmatrix}
    x_1 & y_1 & z_1 & 1 \\
    x_2 & y_2 & z_2 & 1 \\
    x_3 & y_3 & z_3 & 1 \\
    x_4 & y_4 & z_4 & 1 \\
    \end{vmatrix},
\end{equation}

where \(x_i, y_i, z_i\) are the coordinates of four vertices of the tetrahedron. It is easy to see that the determinant \(d\) can be either positive or negative because of changing the order of the vertices results in swapping a pair of rows in the determinant resulting in the change of its sign. Each determinant \(d\) in the tessellation can be made positive at the initial time. Thus the volume of every tetrahedron becomes \(V_i = d_i/6\). The order of vertices remains intact in each tetrahedron in the course of the simulation.

In the course of time a vertex of a tetrahedron can cross the opposite face. This results in the change of the sign of \(d\) indicating that the tetrahedron has turned inside out. If two neighboring tetrahedra sharing a common face have opposite signs of \(d\) then the common face is an element of the caustic surface and thus becomes a cell in the triangulation of the caustic surface. The caustics identified by this method are A2 singularities according to Arnold’s classification. All higher order singularities are singular lines and points on caustic surface A2. For instance, cusps are A3 singularities on the curves lying on the surface A2.

In our code the determinant \(d\) is calculated for all tetrahedra only at every output time but not at every time step of the simulation. Therefore the numbers of the tetrahedra’s flip-flops are not available. However, finding the triangle elements of caustics requires only the signs of the tetrahedra volumes. Hence, the caustics can be obtained without recording the whole history of flip-flopping. Instead of computing flip-flops of tetrahedra we do it on particles because it is easier to implement numerically at every time step [18]. Obviously there is some inconsistency in this approach but fortunately its effect is tolerable.

Identifying caustics in Eulerian space is getting complicated because they often cross each other. If the number of flip-flops was known for each tetrahedron then caustic triangles could be assigned the mean number of flip-flops of two parent tetrahedra as a proxy assisting the search of caustic surfaces. The caustic elements carrying the same half-integer flip-flop tag would be separated out as an individual caustic surface. But we compute flip-flops only on the vertices of caustic triangles. In order to relieve this problem we have devised two diagnostics.

Anticipating the number of flip-flops to grow from external to internal caustics we assign the mean number of flip-flops computed on the vertices of the caustic triangles \(n_{\Delta} = 1/3 \sum_{i=1}^{3} n_{\Delta}(v_i)\) to the triangles as a diagnostic helping to isolate caustics of different generations. We also expected that the triangles of the internal caustics must be on average smaller by size. In both cases this turns out to be correct as figure 2 demonstrates. We compute the length of the triangle edges \(l_1, l_2, l_3\) and order them as long, medium and short: \(l_L > l_M > l_S\). Three panels with coloured backgrounds show the cdfs of \(l_L, l_M\) and \(l_S\) for twelve levels of \(n_{\Delta}\) in the range from \(n_{\Delta} = 0\) to 6. All cdfs monotonically evolve toward smaller lengths with the growth of \(n_{\Delta}\). This indicates that the caustic triangles are shrinking in ongoing nonlinear evolution. The cdfs of the medium edges \(l_M\) are omitted in figure 2 for visual clarity.
Figure 2. The cumulative probability functions of the longest (solid lines) and shortest edges (dashed lines) of caustic triangles are shown in three panels with colored background. The curves correspond to the caustic triangles with various values of \( n_{\text{ff}}^{\Delta} \) as shown by the labels. The panel with white background shows the median values of long, medium and short edges of the caustic triangles as a function of \( n_{\text{ff}}^{\Delta} \) by the solid lines as specified in the legend. Three dashed lines denote the ratios of the three median values. The units on the horizontal in the colored panels and the vertical in the white panel are Mpc/h. (Incidentally the range of the dimensionless ratios on logarithmic scale fit to the range of the edge lengths.)

Our tessellation decomposes each elementary cube in five tetrahedra [9]. There are two kinds of tetrahedra in Lagrangian space: the central one with volume \( V_c = l_0^3/3 \) and four corner tetrahedra with volumes \( V = l_0^3/6 \) where \( l_0 = L/N_p \approx 0.39 \). Initially the central tetrahedron is regular with edges \( l_C = \sqrt{2} l_0 \). Four equal corner tetrahedra have three edges of length \( l_1 = l_0 \) and three of length \( l_2 = \sqrt{2} l_0 \).

Figure 2 also shows the median values for three edges of the caustic triangles \( M(l_L) \), \( M(l_M) \) and \( M(l_S) \) as a function of \( n_{\text{ff}}^{\Delta} \). As expected each function systematically decreases (on average) with increasing \( n_{\text{ff}}^{\Delta} \). However, there are a few interesting features in the shapes of these functions. The ratio \( M(l_M)/M(l_L) \) shown by the green dashed line in the bottom-right panel is approximately constant (mean = 0.76 and std = 0.04). Probably this indicates that using three side-lengths has some degeneracies.

It is worth noting a simultaneous sharp drop of both \( M(l_L) \) and \( M(l_M) \) between \( n_{\text{ff}}^{\Delta} = 11/3 \) and 4: \( M(l_L) \) approximately from 0.77 \( l_0 \) to 0.21 \( l_0 \) and \( M(l_M) \) from 0.56 \( l_0 \) to 0.18 \( l_0 \). The function \( M(l_S) \) (solid blue) is decreasing faster than \( M(l_L) \) and \( M(l_M) \) (solid red and green respectively) in a range \( 0 \leq n_{\text{ff}}^{\Delta} < 4 \). But after the drop all three functions evolve more evenly as the dashed lines show in a range \( 4 \leq n_{\text{ff}}^{\Delta} < 6 \). Obviously it is only a hint, however, if it is confirmed in more realistic N-body simulations some of these features of the caustic
elements may be useful for the analysis of the caustic geometry. For instance, in this N-body simulation the caustics triangles with \( n_{\Delta} = 4 \) become more compact and smaller that may signal about emergence of compact caustic surfaces surrounding halos.

5 Caustics in a high sampling simulation

We discuss only the final stage of the simulation corresponding to \( a = 1 (z = 0) \) and focus on the structure that has reached the most advanced stage in dynamical evolution. The caustic surfaces in the full simulation box are shown in figure 3. There are only a few largest caustic structures with more than a thousand of caustic elements i.e. caustic triangles/cells and caustic vertices/particles. However, the overall abundance of structures is not much different from that in the HDM simulations in [39].

The geometry of the external caustic shells separating a multi-stream regions from the single-stream region is typically simpler than that of the internal caustics. They resemble the typical caustic structures in the ZA simulations. The internal caustics are much more complex and their shapes have not been systematically studied in cosmological N-body simulations. Identifying and examining some of them is the major goal of our study.

The most dynamically advanced part of the caustic structure in this simulation is highlighted by color in figure 3. It consists of a filament and two haloes at both ends resembling
Figure 4. Four images of the structure highlighted by colour in figure 3. It is rendered with different sampling densities parameterized by the ratio of the Nyquist frequency to the cutoff scale $\kappa = k_{\text{Ny}}/k_c$. Top left: $\kappa = 32$. Top right: $\kappa = 16$. Bottom left: $\kappa = 8$. Bottom right: $\kappa = 4$. Colour encodes the number of flip-flops passed by each particle as indicated by the legend. Only particles that passed at least one flip-flop are shown.

A dumbbell. It is embedded in the external cylindrical caustic with significantly greater diameter than the internal filament.

5.1 Why do we need a high mass resolution simulation?

A short answer is trivial: it is impossible to render or characterize a complex geometry with insufficient number of elements. Long time ago it was shown in two-dimensional high-resolution simulations that the complexity of the structure can be revealed only with sufficiently high mass resolution [31]. Using a tetrahedral tessellation of the three-dimensional manifold allows to improve rendering the DM density with more numerous tetrahedra centers that discloses the structure in considerably more detail [9, 10]. Moreover by exploiting this technique it is possible to devise an improved particle-mesh technique [8, 11, 13]. The new technique allows to follow the evolution even in regions with very strong mixing.

Figure 4 provides a visual illustration of the importance of mass resolution by showing exactly same structure rendered with different number of particles. It is useful to look at the ratio of the cutoff scale to the mass resolution scale $\kappa = k_{\text{Ny}}/k_c$ where $k_{\text{Ny}} = (N/2)(2\pi/L)$ is the Nyquist frequency and $k_c = 4(2\pi/L)$ is the cutoff wave number. The top panels correspond to $\kappa = 32$ and 16 on the left and right side respectively the bottom panels to $\kappa = 8$ and 4 on the left- and right-hand side respectively. The rich structure in the top-left panel ($\kappa = 32$) is steadily fading-out as $\kappa$ is decreasing. Only two weak remnants of the haloes at both ends of the green filament can be identified in the bottom-right panel corresponding
to $\kappa = 4$. In the majority of cosmological N-body simulations of the CDM universe the cutoff of initial power spectrum happens naturally at $\kappa \sim 1$.

5.2 Caustics in two-dimensional slices

First, we demonstrate that the structure shown in figure 3 is a set of physical surfaces. Each caustic triangle is found and plotted independently of all the rest. An assumption that a set of independent triangles represents continuous surfaces inevitably leads to the prediction that the cross-section of a plane with this set of triangles must be a discrete set of continuous lines. Two orthogonal infinitesimal slices through the coloured region in figure 3 are shown in figure 5. The figure unambiguously confirms that the built caustics are true surfaces.

Furthermore, figure 5 confirms anti-correlation between $l_L$ and $n^\Delta_{ff}$ anticipated in section 4. Two left panels show the same infinitesimal slice through both red blobs in figure 3. While two panels on the right-hand side show the slice across the cylindrical filament approximately in the middle between the red blobs. Colour encodes $n^\Delta_{ff}$ and $l_L$ in the top and bottom panel respectively as indicated by the colour bar. It is intriguing that the two-dimensional structure shown in the left panels is remarkably similar to figure 4 obtained in a high resolution two-dimensional N-body simulation [31]. This is suggesting that there are some similar types of caustic structures in both 2D and 3D. However the number of topological types of caustics in 3D is of course greater than in 2D.

Two panels on the right of figure 5 reveal two remarkably smooth concentric ovals. The comparison of the caustic contours in the left- and right-hand side of the figure indicates that the caustic surfaces represent two smooth approximately coaxial oval cylinders in three-dimensional space. Two small closed loops in yellow in the top left panel of figure 5 show the cut through the haloes at both ends of the internal cylindrical caustic which is the boundary of a filament. They are also seen in the bottom left panel in blue. These types of caustic structures (cylindrical and compact closed) do not exist in the ZA. The quasi-cylindrical caustic with two compact closed caustics at both ends resemble a dumbbell. It will be discussed in more detail in section 6. The patterns of caustics in Eulerian planes, particularly around the compact blobs are more cumbersome than that in Lagrangian space as illustrated in section 5.3.2.

The colours in figure 5 can be used as a guidance for qualitative description of particle’s journey from caustic to caustic. This is possible because $n^\Delta_{ff}$ is a monotonically growing function of time for each caustic triangle. As an example we consider the top-right panel of figure 5. A dark blue irregular star-like contour consists of the particles experiencing the first caustic metamorphose. The large cyan oval is made up from particles undergoing the second caustic event. The small star-like caustic near the center is composed of the particles going through the third caustic collapse. Finally, the small oval near the center created by the particles have reached the fourth flip-flop. It is worth stressing that all four caustic collapses have taken place along the directions parallel to the two-dimensional slice and as a result a compact caustic shell has not emerged yet as it has been argued in [8, 19, 20]. The fifth collapse in the orthogonal direction results in the formation of two compact caustic shells seen in the top left panel of figure 5. This will be discussed in detail in section 6.

5.3 Shapes of caustics in three-dimensions

The caustic that are discussed in this paper are certainly only coarse-grained approximations. However, it is worth stressing that even coarse-grained caustics are truly real physical objects although up to the accuracy of a physical model. Therefore caustics must be distinguished
Figure 5. Caustics in two razor thin mutually orthogonal slices of the highlighted region in figure 3 and 4. Left: a slice passing through two yellow halos in figure 4. Right: a slice across the middle of the green filament in figure 4. Colour encodes \( n^{\Delta}_{ff} \) and \( l_L \) in the top and bottom panel respectively. Note that the linear scales are different: the distance between the halo shells (top: light brown, bottom: blue) in the left panels is about 10 Mpc/h while the diameter of the external oval in the right panels is about 5.5 Mpc/h. The longest sides of the caustic triangles used in the colour scale in the bottom panels in dimensionless form \( l_L/l_0 \). Thus, the blue and red ends colours correspond to \( l_L \leq 0.12 \) Mpc/h and \( l_L \geq 0.55 \) Mpc/h respectively.

from contour plots of the density fields because contour levels can be arbitrarily chosen whereas caustics are unambiguously determined by \( n_{str}(x) \) or \( n_{ff}(q) \) fields. A distribution of caustics in space represents a specific intermittent phenomenon. It is a physical system that has only two states: one is a discrete set of caustic surfaces and the rest is empty space. Alternatively it can be considered as a purely geometric structure made up by two-dimensional surfaces. Both require very specific methods of analysis. The caustics change their positions with time but physical velocities of the particles — the vertices of the triangulated surface — cannot be considered as the velocities of a caustic element i.e. a vertex or triangle.
Figure 6. Four images of the caustics in the highlighted part of figure 3. Five caustic shells are shown in blue, magenta, green, yellow and red. The surfaces in blue and magenta are the outermost caustics in the region. Two lower images have been zoomed in. The distance between the red halo shells seen at the bottom right is about ten Mpc/h.

5.3.1 Eulerian space

As we mentioned earlier in our approach the caustic surfaces consist of mutually independent triangles each of which is fully defined by two neighboring tetrahedra. The colored patch in figure 3 is magnified and dissected into five distinct patterns displayed in figure 6. Figure 5 gives the impression that setting thresholds on $n_{\text{ff}}$ and/or $l_L$ may help to isolate particular parts of the entire caustic surface. Each pattern shown in figure 6 is specified by three or four components selected by a single value of $n_{\text{ff}}$ however, the dominant inputs are given by its single value, see table A in appendix A. Two shells in blue and magenta shown in two upper panels are the outermost caustics in the highlighted region in figure 3. The upper right image shows that the caustics in blue and magenta cross each other. In this image the blue caustic is painted with low opacity that allows to better see the caustic in magenta. The middle part of the caustic in magenta looks roughly as a cylinder or tube. The cross section plane passing through its axis gives an idea of its three-dimensional contour (see two left panels of figure 5). The internal caustic in green is displayed in the bottom left panel of figure 6 together with the caustic in magenta which is shown with low opacity. Two red caustics at the bottom
Figure 7. Four images on the left are the caustics in a spherical clip with the radius about 26 Mpc/h in Lagrangian space. They correspond to the caustics in figure 6. Two right panels show a razor thin slice through the full set of caustics in Lagrangian space roughly corresponding to the slice in the left of figure 5. Note the nesting structure of the caustic surfaces in Lagrangian space.

right are compact closed surfaces which are neither spherical nor ellipsoidal. Located exactly at the opposite ends of the yellow tube they form a configuration resembling a dumbbell. The red halos are separated by the distance of approximately ten Mpc/h. We are suggesting that the red caustics would be good candidates for the outermost caustic of the haloes that could be called ‘splashback caustics’ on cluster scales in analogy with ‘splashback radii’ on galactic scales [27, 28, 30]. We provide additional arguments in section 6 where we discuss the velocity fields as well as kinetic and potential energies of one of them.

The dumbbell structure is located inside of green and blue shells in figure 6 which look more familiar since they resemble some of the caustics predicted by the ZA. They are probably formed by the streams falling with the velocities mostly acquired in the large-scale gravitational potential.

There are small caustic structures of the next generation with higher values of $n_{\Delta}^{\Delta}$ which are located within the red caustics. Their shapes are resembling the Zeldovich pancakes with thickness around 0.15 Mpc/h. The thickness is less than the force softening scale therefore their shapes may be artefacts of the insufficient force resolution.

5.3.2 Lagrangian space

The Lagrangian progenitors of five caustic shells displayed in figure 6 are shown in figure 7. In addition, two black caustic shells can also be seen inside the red caustics. The figure confirms the hint offered at the end of section 5.2 that the caustics surfaces in Lagrangian space are easier to disentangle than in Eulerian space. This is because they form a nesting structure in Lagrangian space. For instance, when we discussed the two-dimensional slices in figure 5 it was mentioned that the caustics with high $n_{\Delta}^{\Delta}$ at the top left and small $l_L$ at the bottom left could not be easily seen because other caustics crowded them in the high density regions. This issue is alleviated in Lagrangian space were caustics do not cross each other as shown in two right panels in figure 7. However, they may have common lines where $\lambda_1(q) = \lambda_2(q)$ or $\lambda_2(q) = \lambda_3(q)$ [24, 25]. Unfortunately, the Lagrangian caustics built up from the triangle faces of the tessellation are rather corrugated.
Figure 8. Left panel: the velocities of the vertices of the external caustic shell shown in figure 6 in magenta. Note that the arrows render only velocity directions. The speeds of particles are encoded by colour. The set of arrows selected by statistically uniform spatial distribution for clarity. Two brown blobs are the halo caustic shells. Brown colour allows better see the high speed particles in red. Right panel: the velocities of the vertices of the internal caustic shell. Note the difference in colour scales.

6 The dumbbell structure

6.1 Velocity streams

First, we consider the physical velocities of the vertices of the caustic triangles shown in magenta (external caustic) and yellow (internal caustic) in figure 6 and also as semitransparent gray surfaces in figure 8. The velocities of particles are shown by a set of arrows attached to a subset of the caustic vertices. For clarity the subset of the vertices was selected according to statistically uniform spatial distribution. Therefore the appearance of the arrows does not reflect the actual density of the caustic vertices. The arrows are of a constant length and the speed is encoded by colour according to the colour bars in the figure. The caustic surfaces in gray are very smooth between the haloes (see also figure 5) but outside they have rather complex connections with other parts of the caustic web. Those are better seen in figure 3.

The velocity patterns are similar in both caustics. They demonstrate the steady growth of velocities toward the haloes. The vector colours change from blue to red according the colour bar. There is a relatively narrow region on both caustics where the longitudinal component of the particle velocities changes the sign indicating the boundary between the zones of gravitational influence of each halo.

6.2 The halo bounded by a caustic

Here we consider the structure of the streams inside one of two brown caustic shells shown in figure 8. The shell is in the left hand side in both images. The caustic is closed and looks approximately convex however, the shape is neither spherical nor ellipsoidal. We begin with the explanation of how the caustic shell and all interior particles have been found.

6.2.1 Building the mask for an asymmetrical halo

The first step was to identify a caustic shell by using threshold on $n_{\Delta}$ according table A. It it shown in the top left panel of figure 9 rendered by ParaView in 3D. The next step was to find all particles inside the shell. In order to do so a three-dimensional mask matching the

\footnote{This is one of standard options in ParaView}
caustic shell has been build as described bellow. In order to speed up computing we begin with selecting all the particles in a small cube of size 3/Mpc that completely encompasses the caustic boundary. The box contains 79563 particles with the total mass $3.9 \times 10^{14} M_\odot/h$.

The image in the top right panel shows the caustic surface and all particles in the box with $n_{ff} \geq 4$. Some particles coloured in black with $n_{ff} = 4$ are outside of the caustic shell but as we will see later the most of such particles are inside. Two images in the bottom panels show the caustic shell and all the particles in the box with $n_{ff} \geq 5$ and $n_{ff} \geq 6$ on the left and right of the figure respectively. Therefore the particles with $n_{ff} \geq 5$ can be used for building the mask that later may be used for selecting particles inside the caustic shell. In our case we map the particles with $n_{ff} \geq 5$ into an auxiliary cubic grid using the nearest-grid-point (NGP) scheme to label the grid points inside the caustic shell. The labeled grid points make the geometrical template for the halo based only on the local value of $n_{ff}$ without additional assumptions. The last step is to identify all particles in the sub-box that are near the mask grid points.

The red, blue and black histograms on the left of figure 10 show the number of particles inside and outside of the caustic boundary as well as the total in the sub-box respectively. The blue histogram — the black histogram minus the red one — clearly shows that there are no particles outside the shell with $n_{ff} \geq 5$. It also shows that the most of particles with $n_{ff} = 4$ are inside the shell. The red histogram shows that the number of particles with
$n_{\text{ff}} = 4$ and $n_{\text{ff}} = 3$ inside the shell is greater than that outside the shell however, if $n_{\text{ff}} < 3$ the opposite is correct. The distribution of the distances of the caustic vertices from the center of mass of the caustic particles shown on the right of figure 10 provides some feeling of its asymmetry.

The total volume of the template region is $V_{\text{templ}} = 2.4\, (\text{Mpc}/h)^3$ which is a good approximation of the volume within the caustic shell. The counts of particles with 7, 6, 5, 4 flip-flops within the caustic shell are 59, 3893, 12158, and 15817 respectively. The total number is 31927 making the mass within the shell $M(n_{\text{ff}} \geq 4) = 1.6 \times 10^{14} M_\odot/h$. However, the shell contains also streams with 0, 1, 2, and 3 flip-flops with 630, 805, 4037, and 7325 particles respectively. Thus, the total number of all particles within the caustic shell is 44724 and the mass becomes $M(0 \leq n_{\text{ff}} \leq 7) \approx 2.2 \times 10^{14} M_\odot/h$. Dividing the mass by the volume within the caustic shell we estimate the mean density within the shell as $9.2 \times 10^{13} M_\odot/h^2/\text{Mpc}^3$ which is about thousand times greater than the mean mass density in the universe.

6.3 Velocity field within the caustic shell

Figure 11 illustrates the velocity fields in the streams selected by the values of flip-flop numbers $n_{\text{ff}}$. All arrows have the same length thus showing only the directions of the velocities of a randomly selected particle set for every stream for clarity. The colour encodes the speed. The discrete set of colors represents equally spaced intervals in the range from the minimum to maximum of the particle speeds as described in the caption to figure 11.

The velocity streams seems to form the patterns of four types.

1. The slowest particles with 7 and 6 flip-flops in the upper left panel show the infall on the pancake-like caustic structure within the caustic boundary.

2. The particles with 5 and 4 flip-flops in the upper right and in the middle left panels seem to relate mostly to the caustic shell of the halo. The particles in magenta in the upper right and blue particles in the middle left panels indicate the decrease speed as they are approaching to the caustic boundary from inside.
Figure 11. Velocities in the streams selected by the flip-flop count $n_{ff}$. Randomly selected subsamples of the particles within the caustic shell are shown in six panels. Top-left panel: $n_{ff} = 7$ or 6. Top-right panel: $n_{ff} = 5$. Middle-left panel: $n_{ff} = 4$. Middle-right panel: $n_{ff} = 3$. Bottom-left panel: $n_{ff} = 2$. Bottom-right panel: $n_{ff} = 1$ or 0. The caustic is shown by semi transparent gray surface. Vectors show only the direction of the velocities. Colour encodes the ranges of speed in km/s: $19 < \text{blue} < 316 < \text{magenta} < 613 < \text{cyan} < 910 < \text{green} < 1206 < \text{yellow} < 1503 < \text{red} < 1800$.

3. Two panels dominated by green arrows in the middle right and the lower left panels seem to fall into the central part and building up another caustic structure with different geometry than the caustic shell.

4. Finally, the fastest particles - yellow and red - in the lower right panel seem to zoom through the caustic shell practically ignoring its gravitational field.

6.4 The energy distribution in the halo

The distribution of particle energies in the halo provides an additional diagnostic of its dynamical structure. We evaluate kinetic, potential and the total energies for all particles in the halo: $K_i = 0.5m_pv_i^2$, $U_i = -Gm_p^2 \sum_{j=1}^{N_p} |\mathbf{r}_i - \mathbf{r}_j|^{-1}$ ($j \neq i$) and $E_i = K_i + U_i$ where $i$ is the numerical label of a particle. In order to be consistent with the simulation we used a similar condition for softening gravity: in cases when the separation of two particles $|\mathbf{r}_i - \mathbf{r}_j|$ is less...
Figure 12. Kinetic and negative potential energies of the particles in the halo are plotted as the functions of the total energy shown on the horizontal in units of $10^{59}$ ergs/h. The streams are indicated by different colours. The coloured dots in the legend are proportional to the sizes of the points in the plots. Stars in black circles show the corresponding mean values for each stream. The blue and red lines connecting the stars show the kinetic and potential energies respectively. The vertical dashed line marks zero of the total energy. The mean energies of the stream with $n_{ff} = 3$ (in green) approximately satisfy the virial ratio.

than the force softening scale $R_s = 0.8 h^{-1}$ Mpc it was enforced to be to $R_s$. The dot plots in figure 12 show the kinetic $K_i$ and negative potential $-U_i$ energies as a function of total $E_i$ energy. The particles in each stream have its own colour. The colour scheme is the same as in figure 11. The mean potential energy is almost identical in every stream. Therefore the relation between the mean total and kinetic energies is almost exactly linear $\langle K \rangle \approx 1.1 + \langle E \rangle$ in units of $10^{59}$ ergs/h.

The mean total energy is steadily decreasing with the grows of the number of flip-flops in the stream. It is negative for streams with $n_{ff} \geq 2$ while $E$ is positive for the streams with $n_{ff} < 2$. The virial ratio is $\langle K \rangle / |\langle U \rangle| \approx 1.6$ and 1.7 for streams with $n_{ff} = 1$ and 0 respectively. The streams with $n_{ff} \leq 1$ are unlikely gravitationally bound to the halo. Therefore their input into the kinetic energy of the halo can be excluded from the total energy, but the input to the potential energy probably should be kept because it is not affected by their speeds.

Direct summation of kinetic energies of all particles results in $K = \sum_i K_i = 1.27 \times 10^{63}$ ergs/h and summation of potential energies over all pairs of particles gives $U = \sum_i U_i = -2.4 \times 10^{63}$ ergs. The ratio $K/|K + U| = 1.12$ that is 12% higher than the perfect virial ratio. The fraction of kinetic energy by two fastest streams with $n_{ff} \leq 1$ is about 13%. Thus if it is excluded from the total energy balance then the ratio become $K/|K + U| = 0.87$ which is 13% less than exact virial ratio. Both seem to be in a reasonable agreement with the virial ratio if one takes into account that both $K$ and $U$ are supposed to be averaged over time and the dynamical system is assumed to be stable. Neither requirement is exactly fulfilled in this case.
Figure 13. Phase space structure of the halo bounded by the caustic shell. Left-hand panel: two streams with $n_{\text{ff}} \leq 1$ (brown and blue) and the boundary particles in cyan. These are the fastest streams in the halo. The gravity of the halo does not noticeably affect these streams. Right-hand panel: five streams with $n_{\text{ff}} \geq 2$. Colour encodes the number of flip-flops in every stream. The vertical dashed line indicates the most distant elements of the caustic shell from the halo center of mass. The horizontal dashed line separates inflow and outflow particles. The sizes of the dots in the colour legend are proportional, though, not equal to the sizes of the dots in the plots.

6.5 The halo phase space

Unfortunately it is not feasible to illustrate of the velocity field in the caustic shell region in the full six-dimensional phase space. Therefore figure 13 presents a commonly used two-dimensional scatter plots of the radial velocity vs. radial distance from the center of mass of the halo. The radial velocity is measured with respect to the mean velocity of the halo. It is worth emphasizing that the halo is at the origination stage therefore its outermost caustic has a rather irregular shape. The panel on the left of figure 13 shows two coloured streams (brown and blue) with $n_{\text{ff}} \leq 1$ as well as the caustic particles in cyan. The range of the radial velocities of the boundary caustic vertices is also quite large. The distribution of particles seems to show little influence of the halo gravity on these streams. For the particles with zero flip-flops (brown) this is the first run inside a multi-stream region after they crossed the blue caustic from outside of the multi-stream region without experiencing a flip-flop. When they reach the caustic between the three-stream flow from the inside of the three-stream region they experience the first flip-flop and return back to the three-stream flow region. Their color changes from brown to blue in the phase space plot. The next metamorphose of some of them happens when they reach from inside the caustic in magenta. However, no particle with $n_{\text{ff}} \leq 1$ that enter the halo is gravitationally bound (see figure 12) to the halo and therefore all of them exit the halo.

The panel on the right-hand side of the figure shows the phase-space structure of the streams that become gravitationally bound to the halo. There are three types of particles entering the halo. All of them experienced a flip-flop event in the caustic in magenta. Then some of them directly enter the halo while another group experiences the second flip-flop event in the green caustic and then enter the halo. The third set of particles also experiences a caustic metamorphose in the yellow caustic and only then enter the halo. There are three streams with $2 \leq n_{\text{ff}} \leq 4$ entering the halo and no particles with $n_{\text{ff}} \geq 2$ leave the halo. Since the caustic metamorphoses results in the growth of flip-flops therefore the particles
in magenta have experienced two flip-flops, green particles three and yellow particles four flip-flops. The red particles have experienced the fifth flip-flop inside the halo and some of them have became black experiencing the sixth and seventh flip-flops.

The phase space pattern shown on the right-hand side of the figure 13 is typical for haloes. The external streams with \(2 \leq n_{ff} \leq 4\) are entering the halo with negative radial velocities. They fall on the central region and after passing it the particles get going away with positive radial velocities. This results in instantaneous leaps of the particles from the lower part onto the upper part in the phase space diagram. The positive radial velocities of the particles are gradually decreasing with the growth of the radial distances. At some distance the fluid elements experience another flip-flop resulting in the formation of the caustic boundary of the halo. Comparing this figure with figure 6 one can anticipate strong anisotropies of the streams entering the halo.

It is worth stressing that the pattern of the phase space shown in figure 13 is strongly affected by the lack of spherical symmetry in the caustic boundary of the halo. It is highlighted by the cyan particles in the left-hand panel of the figure. The caustic boundary operates as a splashback shell described in [28] who stressed that “the splashback shells are generally highly aspherical, with non-ellipsoidal oval shapes being particularly common”.

7 Fitting the halo boundary by a convex hull

In this section we explore the shapes of two haloes shown in figure 8. The physical features of one of them have been discussed in section 6. Both are neither spherical nor ellipsoidal which are mostly used in the studies of DM haloes. The next relatively simple but considerably more general set of shapes is a class of convex polyhedra. A convex hull perfectly approximates ellipsoids as well as arbitrary convex surfaces with sufficient number of faces Thus, this section describes an attempt to fit the boundaries of two haloes by convex hulls and relate them to the caustics constructed in this simulation.

7.1 Fitting the halo template

The halo has been cut into sixteen two-dimensional slices along three orthogonal axes in both Eulerian and Lagrangian spaces. Then the boundary of a cloud of particles in each slice was compared with the convex hull constructed on these particles.

We first discuss Eulerian space shown in figure 14. The halo template extends over 1.3, 1.7 and 1.8 Mpc/h in \(x\), \(y\) and \(z\) directions respectively. In order to prevent the images from geometrical distortions they are plotted in equal squares of 1.9 by 1.9 Mpc/h. The thickness of slices is about 0.12 Mpc/h and thus the halo occupies 11, 14 and 15 slices in \(x\), \(y\) and \(z\) directions respectively. All 40 slices have been evaluated and plotted. In addition, the two-dimensional convex hull is built and plotted in each slice. Fifteen approximately equally spaced slices are shown in figure 14. A visual inspection of all forty slices has shown no significant difference in the quality of the fit compared to fifteen slices shown in the figure.

A similar approach is also used for the evaluation the quality of convex hull fitting the progenitor boundary in Lagrangian space as shown in figure 15. The only difference is that the particles are distributed on a regular grid. The progenitor of the halo extends over approximately 4, 5 and 6 Mpc/h in \(x\), \(y\), and \(z\) directions respectively. The thickness of slices is about 0.39 Mpc/h and thus the halo occupies 10, 13 and 15 slices in \(x\), \(y\) and \(z\) directions respectively. All 38 slices have been evaluated and plotted. Fifteen approximately equally spaced slices are shown in figure 15.
Figure 14. Five slices of the halo which are parallel to the Cartesian axes shown in each panel are plotted in Eulerian space. The thickness of each slice is about 0.12 Mpc/h. The size of the cube shown in the plots is 1.9 Mpc/h. Black dots are the particles with \( n_{ff} \geq 5 \) projected on the corresponding plane. The two-dimensional convex hulls are shown by red lines. Red points are the vertices of the hulls.

Figure 15. Slices of the halo orthogonal to the three Cartesian axes are plotted in Lagrangian space. The thickness of slices is 0.39 Mpc/h. The size of the cube shown in the plots is about 6 Mpc/h. Black dots are the particles with \( n_{ff} \geq 5 \) projected on a plane. The two-dimensional convex hulls are shown by red lines. Red points are the vertices of the hulls.

We conclude that the boundary of this halo is remarkably well approximated by a convex hull in both Eulerian and Lagrangian space.

7.2 Two convex hull approximations of a halo boundary

There are two somewhat different sets of particles to construct a convex hull from. One of them uses the vertices of the caustic triangles. The other set consists of all particles in the halo with lowest \( n_{ff} \) as illustrated in figure 9.

As it has already mentioned the boundary of a Delaunay tessellation is a convex hull. Therefore it can be used for illustrations of convex hull geometry. As an example we consider
Figure 16. Three mutually orthogonal razor thin slices through the Delaunay tessellations D11 and D12 of the halo shown in figures 8 and 9. D11 and D12 are shown as a filled contour as a black wireframe respectively.

Figure 17. Three slices through the Delaunay tessellations D21 and D22 of the other halo in the dumbbell shown on the right-hand sides of both panels in figure 8.

The Delaunay tessellations of both halos that were earlier shown in Lagrangian space in figure 7 and in Eulerian space in figure 8.

The first Delaunay tessellation D11 is constructed from vertices of the caustic triangles that satisfy two conditions $4 \leq n_{ff}^{\Delta} \leq 14/3$ and $t_L > 0.49 \text{ Mpc/h}$ within a sphere with the center at $r_1 = (47.4, 38.8, 56.4) \text{ Mpc/h}$ and radius $R_1 = 1.1 \text{ Mpc/h}$. The second tessellation D12 is build on particles with $n_{ff} = 5$ contained within the same sphere. Three razor thin slices of both tessellations are shown in figure 16. The slices lie in the mutually orthogonal planes. The plane cuts through the Delaunay tessellation look like wireframes. We focus on the boundaries only which are convex hulls. The filled and wireframe contours correspond to D11 and D12 tessellations respectively. The convex hulls look remarkably similar, however the boundary built on the caustic vertices extends a little further from the center in most parts. This is not surprising because all wireframe vertices are with $n_{ff} = 5$ while some of the caustic vertices are with lower values of $n_{ff}$.

Figure 17 shows similar slices of the Delaunay tessellations D21 and D22 of the other halo seen on the right-hand sides in both panels of figure 8. The vertices of D21 triangulation satisfy a condition $13/3 \leq n_{ff}^{\Delta} \leq 14/3$. The black wireframe corresponds to the particles with $n_{ff} = 5$. Both are selected within a sphere with the center at $r_2 = (38.2, 40.7, 59.6) \text{ Mpc/h}$ and radius $R_2 = 1.2 \text{ Mpc/h}$. Both convex hulls demonstrate a remarkable similarity comparably to the first halo.

We therefore conclude that the caustic boundaries of both halos constructed by two different approaches are in a very good agreement. As expected the convex hull built on caustic vertices is slightly greater than one built on the particles selected by a critical flip-
flop number threshold $n_{ff}$. In addition, the typical separation of two convex hulls is less than the size of the most triangles in the parent Delaunay tessellations. This provides additional robustness to the result.

These results look encouraging for improving and further development this technique. In particular, applying this method to more realistic simulations i.e. greater sample haloes, longer evolution in the non-linear regime

8 Summary

The most common approach to the study of the DM structures consists in the analysis of the DM density field and the velocities of particles in cosmological N-body simulations. We are suggesting a complimentary technique based on identifying and exploring the caustic surfaces and flip-flop counts. The caustic positions in space as well as their shapes are completely determined by $n_{str}(x)$ and $n_{ff}(q)$ fields which differ significantly from the density field and thus to further help in extracting physical insights from N-body simulations. In N-body simulations caustics are built by triangles of the tessellation of the Lagrangian manifold $x(q,t)$.

It is worth stressing that the caustics in our simulation can not be associated with fine-grained phase space streams. However, the estimate of the DM density from N-body simulations is also only a coarse-grained field. Thus the caustics in N-body simulations should be considered as the coarse-grained approximation obtained from a coarse-grained phase space. As such these results can not be directly used for the estimates of the density in the fine-grained caustics. On the other hand we show that the coarse-grained caustics can provide a reasonably good approximation for boundaries of DM haloes.

This work is based on the analysis of the flip-flop field $n_{ff}(q)$ evaluated in Lagrangian space on all particles at each time step by numerical estimating the Jacobian $J(q,t) = \det(\partial x_i/\partial q_j)$. In addition, two auxiliary parameters $n_{ff}^\Delta$ and $l_L$ (see section 4) are used to better identify caustic triangles required for building the halo caustic boundary.

Our major findings are summarized bellow.

1. Defining a caustic element as the common triangle face between neighboring tetrahedra with opposite parities we have constructed caustic surfaces on particles in N-body simulations. Furthermore, we have identified six geometrically and topologically different caustic surfaces in an idealized N-body simulation, see figure 6.

2. We have identified the caustic structure resembling a dumbbell. It consists of two halo shells connected by a quasi-cylinder caustic, see figure 8. Many examples of this structure can be seen in the density plots in [10, 27, 40], however, with significantly lower resolution. In our idealized simulation the dumbbell structure is coaxially embedded into another quasi-cylindrical caustic with roughly three times greater diameter. The velocity patterns in both internal and external cylindrical caustics suggest that the particles are approaching the haloes with increasing speed. This is an agreement with the prediction made long ago, see e.g. [3]. Finding this structure in a small simulation suggests that despite very idealized initial conditions it yields such a generic structure.

3. We have shown how to identify the halo boundary by setting a threshold on $n_{ff}(q) \geq n_{cr}$. Due to discrete nature of the flip-flop counts there may be a rapid transition between the geometry and topology of the streams differed by a single flip-flop as figure 6.
demonstrates. Using the count of flip-flops on particles as a threshold parameter we have constructed two haloes by selecting the particles with $n_{ff}(q) = 5$. The streams with $n_{ff}(q) > 5$ are fully inside of the halo boundary while those with $n_{ff}(q) < 5$ have only a small fraction of particles within the boundary. Taking one of the haloes as an example we illustrated the idea of the method. We constructed a template of the halo geometry based on the stream with $n_{ff}(q) = 5$ without making any assumption about its shape. By using the template all particles with $n_{ff}(q) < 5$ have been identified as the members of the halo. The analysis of kinetic and potential energies of the particles in the individual streams within the halo boundary has shown that only the particles with $n_{ff} \geq 2$ are gravitationally bound, see figure 12. An examination of the halo phase-space also confirms this conclusion.

4. The convexity of the halo template in Eulerian space was tested and confirmed. An analogous test carried out on the progenitor of the halo in Lagrangian space has shown a similar result. Based on this result we compared two convex hulls constructed on different set of particles. One set of particles was selected by imposing a threshold on $n_{ff}$. The second was constructed using the vertices of the compact caustic surrounding the halo. Three mutually orthogonal razor thin slices were cut for both halos. They show a very good agreement between both convex hulls in both halos, see figures 16 and 17. Based on the reported results it seems reasonable to suggest that the boundaries of many dark matter halos can be associated with the outmost caustic that enclose only that one halo, but no other halo. The goal of this approach is similar to the one of [27, 28], however, the numerical techniques are significantly different. The caustic surfaces themselves are not necessary all convex but some certainly are, in particular, the haloes which are not in the merging process. It is worth stressing that the haloes studied in this paper belong to the first generation of haloes. They neither have experienced hierarchical structure formation nor have substructure in the form of subhaloes. The limitations of the N-body simulation used in this study may cast doubt on the relevance of the reported results to the simulations with sufficient small-scale power in the initial power spectrum.

We are looking forward to carry out a more detailed analysis on higher resolution simulations. In particular, because the detailed analysis of the 3D structures of 906 splashback shells with number of particles $N_{200m} > 50,000$ and a clear steepening of the density profile in their outskirts obtained from the suite of large N-body simulations concluded that splashback shells are generally highly aspherical, with non-ellipsoidal oval shapes being particularly common [28].

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A Identifying distinct caustic structures

A caustic element — a caustic triangle and its vertices — is defined as the shared face of a pair of neighboring tetrahedra having opposite signs of volumes evaluated by Equation 4.1. Each caustic triangle is treated as an independent entity. Therefore the caustic surfaces can
be completely determined by a local condition. The mean value of the flip-flop counts on three vertices of a caustic triangle is discrete: $n_{\Delta} = n \times (1/3)$ ($n$ — integer) because the number of counts of flip-flops on each vertex is integer. The number of the caustic elements for each value of $n_{\Delta}$ is given in table A. The table also provides the reference to the colour of five caustics shown in figure 5. Two innermost caustics can be seen only in Lagrangian space shown as black blob inside red caustic shells in figure 7.

Table 1 shows that the most of triangles with $n_{\Delta} = 1$ are in the caustic in magenta but about 10% of them belong to the blue caustic. Similarly the majority of triangles with $n_{\Delta} = 2$ are in the green caustic but about 10% belong the caustic in magenta. Probably it is caused by inconsistency between counting flip-flops on vertices of the tessellation tetrahedra and identifying the caustic triangles by comparing parities of the tetrahedra themselves. We leave solving this problem for the further work.

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