MASS OF CLUSTERS IN SIMULATIONS

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Received 2002 May 2; accepted 2003 January 9

ABSTRACT

We show that dark matter halos in N-body simulations have a boundary layer (BL), which neatly separates dynamically bound mass from unbound materials. We define $T(r)$ and $W(r)$ as the differential kinetic and potential energy of halos and evaluate them in spherical shells. We notice that in simulated halos such differential quantities fulfill the following properties: (1) the differential virial ratio $\mathcal{A} = -2T/W$ has at least one persistent (resolution-independent) minimum $r_c$ such that, close to $r_c$, (2) the function $w = -d\log W/d\log r$ has a maximum, while (3) the relation $\mathcal{A}(r) \simeq w(r)$ holds. BLs are set where these three properties are fulfilled, in halos found in simulations of "tilted" Einstein–de Sitter and ΛCDM models, run ad hoc, using the ART and GADGET codes; their presence is confirmed in larger simulations of the same models with a lower level of resolution. Here we find that ~97% of the ~300 clusters (per model) we have with $M > 4.2 \times 10^{14} h^{-1} M_\odot$ own a BL. Those clusters that appear not to have a BL are seen to be undergoing major merging processes and to grossly violate spherical symmetry. The radius $r_c$ has significant properties. First of all, the mass $M_r$ it encloses almost coincides with the mass $M_{\text{dyn}}$, evaluated from the velocities of all particles within $r_c$, according to the virial theorem. Also, materials at $r > r_c$ are shown not be in virial equilibrium. Using $r_c$ we can then determine an individual density contrast $\Delta_c$ for each virialized halo, which we compare with the "virial" density contrast $\Delta_v \simeq 178 \Omega_m^{0.45}$ (where $\Omega_m$ is the matter density parameter) obtained assuming a spherically symmetric and unperturbed fluctuation growth. As expected, for each mass scale, $\Delta_c$ is within the range of values $\Delta_v$. However, the spread in $\Delta_c$ is wide, while the average $\Delta_c$ is ~25% smaller than the corresponding $\Delta_v$. We argue that the matching of properties derived under the assumption of spherical symmetry must be a consequence of an approximate sphericity, after violent relaxation destroyed features related to ellipsoidal nonlinear growth. On the contrary, the spread of the final $\Delta_c$ is an imprint of the different initial three-dimensional geometries of fluctuations and of the variable environment during their collapse, as suggested by a comparison of our results with the Sheth & Tormen analysis.

Subject headings: cosmology: theory — dark matter — galaxies: clusters: general — large-scale structure of universe — methods: N-body simulations

On-line material: color figures

1. INTRODUCTION

The inner region of dark matter halos in N-body simulations is certainly virialized. A precise detection of the boundaries of such a region, however, is a long-lasting and not yet completely solved problem. If we try just to identify a "collapsed" region, i.e., a region detached from the cosmological expansion, the task is easier (see, e.g., Monaco & Murante 1999 and references therein). However, in general, a collapsed region is not yet in virial equilibrium. The point is that, in a cosmological context, each structure is embedded in a more or less homogeneous background, and we pass gradually from the inner halo to external materials. The aim of this work is to show a precise criterion able to find virialized regions in dark matter halos. This criterion will be tested on simulations and found to be more efficient than previously adopted rules.

As a matter of fact, several global properties of galaxy clusters, such as mass ($M$), radius ($r$), and, also, temperature ($T_X$) or luminosity ($L_X$) are strictly linked to the achievement of equilibrium. Analytical predictions about such global quantities were performed assuming that structures evolve from uniform, spherically symmetric fluctuations, preserve such symmetries during their growth, and feel no influence from their environment (Gott & Rees 1975; Peebles 1980). However, even under such simplifying conditions, a cosmological constant is a significant complication. Lahav et al. (1991) studied the growth of uniform spherical fluctuations within such a context. They also outlined that the most direct way through which observations can distinguish among flat models with different $\Omega_m$ (matter density parameter) is to compare cluster abundances at low and high redshifts. The dynamics of the spherically symmetric growth of a uniform density fluctuation, in a model with $\Omega_m + \Omega_A = 1$ (where $\Omega_A$ is the vacuum density parameter), was further explored by Eke, Cole, & Frenk (1996). Brian & Norman (1998) gave a polynomial expression for the expected density contrast of virialized clusters, which reads $\Delta_c = A + Bx + Cx^2$, with $x = \Omega_m - 1$, and $A = 18\pi^2 \approx 178$, $B = 82$, $C = -39$, and holds at any redshift $z$; this relation is well approximated by the expression

$$\Delta_c = A \Omega_m^{0.45}. \quad (1.1)$$

Under the same assumptions, using a Press & Schechter (1974) approximation, one can predict the expected mass function of clusters.

The impact of this approximation on the estimate of cluster global quantities could be appreciated only through numerical simulations. Much work was therefore devoted
to this aim (see, e.g., Lacey & Cole 1993, 1994; Cole & Lacey 1996; Carlberg et al. 1996; Eke et al. 1996; Eke, Natarro, & Frenk 1998; Brian & Norman 1998; Gardini, Murante, & Bonometto 1999). However, in the very analysis of the numerical work, the above approximations were often implicit. An example is the identification of dark halos based on spherical overdensity (SO) algorithms, with reference to the density contrast $\Delta_c$, given in equation (1.1). In this work we shall also use an SO algorithm (described below) as a selection criterion. However, using equation (1.1), to work out values for the cluster radius ($r_c$) or mass ($M_c$), implies a bias. The values of equation (1.1) are obtained under precise restrictions and numerical work should also verify their impact. In a sense, the problem is even more severe when the values of equation (1.1) are used to define virialized halos without requiring explicitly that they are spherical.

In this work we plan to find a rule, suitable for defining virialized systems, taking into account that a variety of growth histories led to different final features of virialized structures. A number of recent papers (Sheth & Tormen 1999, 2002; Sheth, Mo, & Tormen 2001) had a similar motivation. They tried to study the growth of primeval fluctuations, taking into account the effect of an ellipsoidal collapse. Then, in order to avoid having the collapse on some axis going to zero, they set up a recipe to freeze it out once it has shrunk by some critical factor. This freeze-out radius is explicitly chosen so that the density contrast at virialization for the whole halo is again $\Delta_c$, as given in equation (1.1), i.e., in spherical growth models. In contrast, in this work the use of $\Delta_c$ to define virialized systems is completely overcome. The point is that the detailed growth history of individual halos, in which different ellipticities and velocity anisotropies played an important role, is not expected to leave major traces on final halo shapes after violent relaxation has occurred during the virialization process (Navarro, Frenk, & White 1997). On the other hand, it may result in a significant spread of the equilibrium density contrasts $\Delta_c$ of individual halos. Therefore, when the virial radius of relaxed objects is sought, deviations from spherical symmetry and velocity anisotropies may not be as important as deviations of $\Delta_c$ from $\Delta_c$.

We expect that the value $\Delta_c$, given by equation (1.1), is within the range of the actual $\Delta_c$ values, but we think that it is important to first test how extended this range is and how $\Delta_c$ is set with respect to actual values. Furthermore, a different $\Delta_c$ implies a different radius and mass ($r_c$ and $M_c$) for each object. Accordingly, we expect that some individual object masses increase and others decrease. We will explore the extent of these changes on galaxy clusters in numerical simulations of critical CDM models and without a cosmological constant. Such changes may have an impact on the mass function (see § 5 and Figs. 13 and 14), while some scaling relations might be significantly altered, for instance, the relation between $M$ and $T_X$.

In order to implement our program, we need a simple and effective rule to identify virialized material in clusters. In trying to find such a rule we discovered a precise regularity in the transition region between material belonging to clusters and the surrounding medium. In fact, the volume occupied by virialized materials is confined by a “boundary layer” (BL), whose depth $\Delta r$ ranges around 50–100 $h^{-1}$ kpc and whose properties fulfill precise analytical prescriptions. Such a BL has been found in $\sim$97% of the clusters in our simulated models and is one of the findings of this work.

The BL is not a physical confinement barrier, and particles can travel outward and inward through it. On the contrary, it confines a volume, where material fulfills precise equilibrium conditions, which cease to hold outside it. Inside the BL itself, the formal condition for virial equilibrium of an isolated system holds, as pressure forces at its upper and lower borders cancel each other; on the BL, kinetic energy has a minimum with respect to potential energy, and matter density is rapidly decreasing. These conditions follow from a precise analytical requirement $R_w$ derived under the assumption of spherical symmetry. This $R_w$ requirement will be only approximately satisfied by halos in simulations, where the halo geometries apparently violate spherical symmetry. We show, however, that normal deviations from a spherical shape in dark matter halos do not prevent them from having a BL.

We explicitly note that we do not force the BL to exist, but we apply the $R_w$ requirement and find it. For this reason, finding the BL is different from finding a given spherical overdensity; the latter always exists when average densities of halos decrease with increasing radii, and this does not imply even an approximately spherical symmetry. On the contrary, we could have bound and relaxed regions that are not confined by a BL: our analysis of numerical simulations shows that this is not the case. There is also a major difference between the $R_w$ requirement we are defining here, and other prescriptions, such as SKID, which defines a halo as the set of all particles gravitationally bound to the halo itself. In fact, bound particles are not guaranteed to belong to virialized zones and may belong to regions that are bound but still unrelaxed.

In this paper we shall first discuss when the BL should exist and introduce the $R_w$ requirement used to detect it. To have significant statistics based on this rule and to confirm its validity requires simulations performed with a large dynamic range, as can only be done by parallel computing.

Finding and situating BLs allows a better evaluation of individual cluster masses, radii, and density contrasts, as well as an analysis of their possible dependence on various physical parameters. The study of the structure of dark matter halos in numerical simulations can also be put on a sounder footing. In previous analyses (see, e.g., Cole & Lacey 1996), the $r$ dependence of the integral virial ratio $-2T(<r)/W(<r)$ was discussed and found not to be “useful for defining the boundaries of the virialized region.” One of the findings of our analysis is precisely the possibility of detecting such a boundary, using the virial ratio for shells instead of spheres. Figure 1 compares integral and differential virial ratios, showing how much more information appears to be contained in the latter [see § 3 for details on how $\mathcal{H}(r)$ points are calculated]. Previous analyses have also stressed halo properties apparently depending “on how groups are identified” (Sheth et al. 2001). The existence of a border, with precise physical properties, separating cluster material lets one overcome any such ambiguity.

It may be also important to remember that according to the definitions given above, in this work $\Delta_c$, $r_c$, and $M_c$ are quantities worked out starting from the fixed density contrast given by equation (1.1), while $\Delta_c$, $r_e$, and $M_e$ are the same quantities when worked out from the setting of the BL around each cluster. Let us also point out that the procedure discussed in this work is not the basis for an alternative
cluster-finding algorithm, such as, e.g., friends-of-friends, SKID, or SO. On the contrary, our analysis assumes that cluster locations are given. Here we give a different prescription for defining the physical dimension of the cluster, not its position.

The plan of the paper is as follows. In § 2 we give suitable information on the simulations used, which were partially run ad hoc, for this work. In §§ 3 and 4 we define the boundary layer BL and discuss how it can be found in simulated clusters. In § 5 we show the results of our work, and in § 6 we discuss them and some future perspectives.

2. MODELS AND N-BODY SIMULATIONS

We use two main sets of simulations, performed with different codes: the parallel AP3M N-body code described in Gardini et al. (1999), the parallel PM ART code developed by Kravtsov, Klypin, & Khokhlov (1997), and the parallel tree code GADGET (Springel, Yoshida, & White 2001).

The code of Gardini et al. (1999) was developed from the serial public AP3M code of Couchman (1991), extending it to different cosmological models and allowing suitable flexibility in particle masses. Using this code, two simulations were performed. The first of them, dealing with a “tilted” Einstein–de Sitter model (hereafter TCDM), has already been considered by Gardini et al. (1999); the normalization of the run was, however, rescaled to yield \( \sigma_8 = 0.55 \) at the final step, instead of \( \sigma_8 = 0.61 \), so that the final abundance of rich clusters is the same for both models at the final epoch (as usual, \( \sigma_8 \) is the mean-square density fluctuation on the scale of 8 h\(^{-1}\) Mpc, \( h \) being the Hubble parameter in units of 100 km s\(^{-1}\) Mpc\(^{-1}\)). The latter simulation dealt with a \( \Lambda \)CDM model, i.e., a flat CDM universe with nonzero cosmological constant and \( \sigma_8 = 1.08 \). In view of recent observational results (see, e.g., Schuecker et al. 2002), these normalizations are both rather high, as a reasonable value for \( \sigma_8 \) in \( \Lambda \)CDM models is \( \sim 0.75 \); however, this has no impact when studying inner cluster dynamical properties.

The above simulations (denoted A and B, respectively) are performed in cubes with sides of 360 h\(^{-1}\) Mpc. CDM+baryons are represented by 180\(^3\) particles, whose individual mass is 2.22 \( \times \) 10\(^{12}\) h\(^{-1}\) \( M_\odot \) for TCDM and 0.777 \( \times \) 10\(^{12}\) h\(^{-1}\) \( M_\odot \) for \( \Lambda \)CDM. We use a 256\(^3\) grid to compute the fast Fourier transforms needed to evaluate the long range contribution to the force (PM), and we allow for mesh refinement where the particle density attains or exceeds \( \sim 30 \) times the mean value. The starting redshifts are \( z_{in} = 10 \) for TCDM and \( z_{in} = 20 \) for \( \Lambda \)CDM. The particle sampling of the density field is obtained by applying the Zeldovich approximation (Zeldovich 1970; Doroshkevich et al. 1980) starting from a regular grid. We adopt the same random phases in both A and B.

The number of steps were 1000 equal \( p \)-time steps (the time parameter is \( p \sim a^{1/3} \), where \( a \) is the expansion factor). The comoving force resolution, given by the softening length, is \( \eta \sim 112 \) h\(^{-1}\) kpc, yielding a Plummer equivalent softening \( \epsilon_P \sim 40.6 \) h\(^{-1}\) kpc. These simulations were described in more detail in Gardini et al. (1999) and were also used in Maccio et al. (2002). The parameters of the models are reported in detail in Table 1.

In order to see how resolution affects the results of the \( R_w \) requirement, we performed further simulations with the ART code (courtesy of A. Klypin). This allows us to select regions inhabited by clusters and to rerun them with increasing particle mass resolution, from 7.7 \( \times \) 10\(^{11}\) \( \Omega_m \) h\(^{-1}\) \( M_\odot \) to 1.2 \( \times \) 10\(^{10}\) \( \Omega_m \) h\(^{-1}\) \( M_\odot \). The ART (Adaptive Refinement Tree) code (Kravtsov et al. 1997; Knebe et al. 2000) starts with a uniform grid, which covers the whole computational box. This grid defines the lowest (zeroth) level of resolution of the simulation. The standard particle-mesh algorithms are used to compute the density and gravitational potential on the zeroth-level mesh. The code then reaches high-force resolution by refining all high-density regions using an automated refinement algorithm. The refinements are recursive: the refined regions can also be refined, each subsequent refinement having half of the previous level’s cell size. This creates a hierarchy of refinement meshes of different resolution, size, and geometry covering regions of interest. Because each individual cubic cell can be refined, the shape of the refinement mesh can be arbitrary and effectively match the geometry of the region of interest. This algorithm is well suited for simulations of a selected region within a large computational box.

### Table 1

| Parameter          | TCDM (A) | \( \Lambda \)CDM (B) |
|--------------------|---------|---------------------|
| \( \Omega_m \)     | 1       | 0.35                |
| \( \Omega_\Lambda \) | 0       | 0.65                |
| \( \Omega_b \times 10^2 \) | 6   | 3.6                 |
| \( n \)            | 0.8     | 1.05                |
| \( h \)            | 0.5     | 0.65                |
| \( \sigma_8 \)     | 0.55    | 1.08                |
| \( \Gamma \)       | 0.32    | 0.19                |
The criterion for refinement is the local density of particles: if the number of particles in a mesh cell (as estimated by the cloud-in-cell method) exceeds the level \( n_{\text{thresh}} \), the cell is split (“refined”) into eight cells of the next refinement level. The refinement threshold may depend on the refinement level. The code uses the expansion parameter \( a \) as the time variable. Besides spatial refinements, during the integration time refinements are also performed.

The ART code can handle particles of different masses. This lets us increase the mass (and correspondingly the force) resolution of regions centered around the highest mass clusters. The multiple-mass resolution is implemented in the following way. We first set up a realization of the initial spectrum of perturbations so that initial conditions for our largest number (512\(^3\)) of particles can be generated in the simulation box. Coordinates and velocities of all the particles are then calculated using all waves ranging from the fundamental mode \( k = 2\pi / L \) to the Nyquist frequency \( k = 2\pi / L \times N^{1/3}/2 \), where \( L \) is the box size and \( N \) is the number of particles in the simulation. We obtained lower resolution regions by merging high-resolution particles into particles of larger mass where needed. This process can be repeated to get still lower resolution. The larger mass (merged) particles have velocities and displacements equal to the average of the velocities and displacements of the smaller mass particles. Using this technique, we first generated initial conditions for low-resolution simulations. These simulations were run from their initial redshift to \( z = 0 \), and they were used to locate the Lagrangian regions forming the most massive clusters. Then, we were able to obtain initial conditions (ICs) at high resolution (in both force and mass) in the selected Lagrangian zones, with the same random Fourier phases. Such zones were surrounded by lower and lower resolution shells, taking into account the tidal field that acts on them. Finally, these ICs were used to run the high-resolution cluster simulations.

The simulations employed here were performed using 128\(^3\) zeroth-level grid in a computational box of 180 \( h^{-1} \) Mpc. The threshold for cell refinement (see above) was low on the zeroth level: \( n_{\text{thresh}}(0) = 2 \). Thus, every zeroth-level cell containing two or more particles was refined. The threshold was higher on deeper levels of refinement: \( n_{\text{thresh}} = 3 \) and \( n_{\text{thresh}} = 4 \) for the first level and higher levels, respectively.

For the low-resolution runs the step in the expansion parameter was chosen to be \( \Delta a_0 = 2 \times 10^{-3} \) on the zeroth level of resolution. This gives about 500 steps for particles located in the zeroth level for an entire run to \( z = 0 \) and 128,000 for particles at the highest level of resolution.

Using the ART code we performed two simulations: a \( \Lambda \)CDM model and a TCDM model, which we will indicate as C and D, respectively. These models are similar, although not identical, to those of Gardini et al. (1999); their parameters are listed in Table 2. We identified the clusters in these zero-level simulations and selected the six largest mass clusters for each cosmological model. They were rerun with increased mass (and force) resolution, using the method described above. For every selected cluster, we have three runs with resolutions\(^4\) of 128\(^3\) (particles mass

\[ M_p = 7.7 \times 10^{11} \Omega_m h^{-1} M_\odot, \]

256\(^3\) \((M_p = 9.6 \times 10^{10}\Omega_m h^{-1} M_\odot)\), and 512\(^3\) \((M_p = 1.2 \times 10^{10}\Omega_m h^{-1} M_\odot)\), with more than 350,000 particles within a radius of 2.0 \( h^{-1} \) Mpc.

We then run three of the six high-resolution \( \Lambda \)CDM clusters with the public parallel tree code GADGET (Springel et al. 2001) to verify that our results do not depend upon the peculiarities of one \( N \)-body code. One of the clusters was magnified with both ART and GADGET. The initial conditions were set as described above. We used a Plummer-equivalent softening length \( \epsilon = 10.98 \); this is also the linear dimension or our highest resolution ART cell. We chose the time-step criterion 3, based on the local dynamical time, with a tolerance of the integration error \( E_{\text{int}} = 0.2 \), which gave us about 100,000 time steps from \( z = 0 \) to \( z = 0 \). The criterion for opening the tree cells is based on the absolute truncation error in the multipole expansion, with a tolerance on the error on the force of \( E_F = 0.02 \) (see Springel et al. 2001 and the code user manual for more details).

In all of our numerical simulations, clusters were identified using a SO algorithm. As a first step, candidate clusters are located by a friend-of-friends algorithm, with linking length \( \lambda = \phi \times d \) (here \( d \) is the average particle separation), keeping groups with more than \( N_f \) particles. We then perform two operations: (1) we find the point, \( C_{\phi} \), where the gravitational potential due to the group of particles is a minimum; (2) we determine the radius, \( r_C \), of a sphere centered in \( C_{\phi} \) in which the density contrast is \( \Delta \). Using all particles in this sphere we perform again the operations 1 and 2. The procedure is iterated until we converge onto a stable particle set. The set is discarded if, at some stage, we have fewer than \( N_f \) particles. If a particle is a potential member of two groups, it is assigned to the more massive one. (Gardini et al. 1999 also describe this SO algorithm in more detail and compare it with other group identification algorithms, e.g., Governato et al. 1999). In this work we set \( \phi = 0.2 \) and take \( N_f \) such that we have a mass threshold 3.0 \( \times 10^{13} h^{-1} M_\odot \). Above this mass threshold there are \( \sim 10,000 \) halos in simulations A and B and \( \sim 1250 \) halos in simulations C and D.

Tests performed by Gardini et al. (1999) show that no cluster is missed above \( 4.2 \times 10^{14} h^{-1} M_\odot \). We have 303 such clusters in A, 316 in B, 40 in C, and 36 in D; six clusters of C and D were then blown up to various resolution levels.

### Table 2

| Parameter | \( \Lambda \)CDM (C) | \( \Omega \)CDM (D) |
|-----------|---------------------|---------------------|
| \( \Omega_m \) | 1                   | 0.3                 |
| \( \Omega_\Lambda \) | 0                   | 0.7                 |
| \( n_h \times 10^2 \) | 5                   | 2.6                 |
| \( n_h \) | 0.8                 | 1.05                |
| \( h \) | 0.55                | 0.7                 |
| \( \sigma_8 \) | 0.55                | 1.08                |
| \( \Gamma \) | 0.31                | 0.21                |

\(^4\) Since our averaging procedure corresponds to using different mesh sizes when generating ICs for a simulation, we will refer to the size of the higher resolution mesh used in each simulation IC when quoting resolutions.

3. THE VIRIAL THEOREM APPLIED TO SINGLE CLUSTERS: THEORY

Finding the volume where cluster materials are in virial equilibrium may seem a tough and somewhat ambiguous task. If kinetic and potential energies, within a radius \( r \), are
defined according to

\[ 2T(< r) = \sum_{i(r<r)} m v_i^2, \]  
\[ W(< r) = - \sum_{i<j(r<r)} G \frac{m_i m_j}{r_{ij}}, \]  

the virial ratio,

\[ \mathcal{R}(< r) = \frac{-2T(< r)}{W(< r)}, \]  

should be unity, in a virialized sphere of radius \( r \), provided that it is fully isolated. On the contrary, in the real world, as well as in simulations, the virialized volume is bordered by infalling and outgoing material, possibly traveling through a partially depleted area. For this reason, the convergence requirement, therefore, goes beyond finding a layer in virial equilibrium. We thus define “boundary layer” as a region satisfying equations (3.11) and (3.12). Unless \( w \) is constant and use equation (3.8) with \( w' = 0 \) and the virial ratio

\[ \mathcal{R}_\Delta = \frac{\sum_{i(r(\Delta r)} m v_i^2 - \int_{\Delta r} \frac{d \mathcal{Z}(r)}{dr}(r)}{\int_{\Delta r} \mathcal{Z}(r)} \]  

to obtain

\[ \mathcal{R} = w, \]  

all along the interval \( \Delta r \). This equation coincides with equation (3.29) in Goldstein, Pole, & Safko (2002) (in turn, the latter equation yields eq. [3.9] above, in the limit \( w \equiv \text{const.} \)).

Requiring that \( w' = 0 \), then, also yields

\[ \frac{d \mathcal{R}}{dr} = 0 \]  

in \( \Delta r \). Conversely, if equations (3.11) and (3.12) are both fulfilled in a layer of depth \( \Delta r \), this layer is at rest and in virial equilibrium. We thus define “boundary layer” as a region of depth \( \Delta r \) satisfying equations (3.11) and (3.12).

Let us stress that requirement 3 is essential to set the \( \dot{R}w \) requirement, defined by equations (3.11) and (3.12). Unless \( w \) is constant along a suitable interval, we can neither replace \( r d \mathcal{Z}(r)/dr \) by \(-w \mathcal{Z}(r)\) in equation (3.9) nor factorize \( w \) out of the sum to obtain equation (3.11). Moreover, should equation (3.11) hold on a single \( r \), we could have \( w' = 0 \) there, with \( \mathcal{R} \neq 0 \). Finding a layer fulfilling the \( \dot{R}w \) requirement, therefore, goes beyond finding a layer in virial equilibrium. As we shall see, however, once the \( \dot{R}w \) requirement is fulfilled, we have found a layer bounding a virialized region.

Let us also stress that the \( \dot{R}w \) requirement does not imply that particles cannot pass through the BL; it only prescribes that such (possible) passages do not violate its stationary conditions. However, if we find about a cluster a boundary layer, it will act as a confinement barrier to inner kinetic and potential energies and mass. Notice that, in principle, inner materials might not be in virial equilibrium themselves; even in this case, however, there can be no net exchange of mass between inside and outside, and the possible energy...
exchange is limited to the work done by tidal torques due to anisotropies.

Let us now show that no further material, outside the BL, can be in virial equilibrium. We will show that this is certainly forbidden if the values, taken by $\mathcal{R}$ and $w$ at $r_+$, are a minimum and a maximum, respectively, when compared with values at $r > r_+$. This simple condition, however, is not strictly necessary; it is sufficient that the difference $\mathcal{R} - w$ increases, becoming positive, at $r > r_+$. This will be shown below. Let us, however, anticipate that, while the $R_w$ requirement can be fairly easily tested, it is not easy to deal with this further requirement. The tests performed on a large number of clusters and described in the next sections, however, let us conjecture that when the $R_w$ requirement is fulfilled, this further requirement is somehow inescapable. We now show why, at $r > r_+$, the equilibrium conditions are violated if a boundary layer is found. Notice that, at $r > r_+$, we can still assume that $W = W(r_+)(r/r_+)^{w}$, but $w$, starting from the value it had in $\Delta r$, will now vary with $r$ and, according to equation (3.8),

$$\mathcal{R} - w = w' \ln(r/r_+);$$

this equation cannot be fulfilled if the difference $\mathcal{R} - w$, vanishing up to $r_+$, increases at $r > r_+$, becoming positive. In fact, we required that $w$ is maximum, and therefore $w' < 0$.

Let us finally notice that if a layer is characterized by higher $w$ values, this means that it is emptier than the inner or outer layers. A maximum of $w$, therefore, indicates a low-density layer. In turn, a minimum of $\mathcal{R}$ indicates a low kinetic energy with respect to potential energy. BLs, therefore, are partially depleted $r$-intervals, where particles, on average, are particularly slow.

4. THE VIRIAL THEOREM APPLIED TO SINGLE CLUSTERS: PRACTICAL USE

The mathematical definition must now be applied to numerical simulations. A failure to find BLs could be attributed to insufficient numerical resolution or to bad violations of spherical symmetry. However, in principle, even if the resolution is enough and no substantial departures from sphericity are visible, BLs could still be absent.

Let us now describe our procedure. After finding clusters in simulations and their centers $C_i$, as described in §2, we evaluated $W(r)$ and $\mathcal{R}(r)$ for spherical $r$-intervals containing a fixed number of particles,

$$N = \frac{M_i}{(2\pi^2 m_p)}$$

(here $M_i$ of the total mass within $4.5 h^{-1}$ Mpc from $C_i$ and $m_p$ is the particle mass). However, successive points along $r$ are obtained by shifting outward by $N/8$ particles. In the relevant $r$ range, the above criterion yields $N \sim 10^2$ for TCDM (simulation A) and $N \sim 3 \times 10^2$ for ΛCDM (simulation B), while successive points lay at a distance $\sim 20 h^{-1}$ kpc. This is below (but not much below) the force resolution ($\sim 100 h^{-1}$ kpc), as desired.

We do not expect BLs to be much thicker than our force resolution; accordingly, we first seek the minima of $\mathcal{R}$. Owing to the procedure by which $\mathcal{R}$ points are worked out, a minimum is considered significant only if it is such with respect to eight neighbors. Finding the maxima of $w$ is harder, as $w(r)$, obtained by differentiating $W(r)$, should then be further differentiated to find its maxima. In practice, however, this second-order differentiation is not needed. Quite in general, there will be just a few points $r_m$ where $\mathcal{R}$ has significant minima. Let then $\mathcal{R}_m$ be the virial ratio at such points and let us fit $W(r)$ with the expression

$$\mathcal{W} = A(r/r_m)^{-\mathcal{R}_m}$$

in $\nu = 8$ points greater than $r_m$, covering an interval $\Delta r \sim 100–150 h^{-1}$ kpc. The fit is performed in two steps: we first minimize the function $\phi = \mathcal{W}/\mathcal{W} - 1$, using only $A$ as a parameter; then, in equation (4.2), we allow $\mathcal{R}_m$ to take values different from the value of $\mathcal{R}$ in $r_m$ and perform a two-parameter fit.

We considered the fit to be satisfactory if two conditions hold: (1) When performing the first fit, the residual

$$\chi^2 = \sum_{i=1}^{\nu} \phi_i^2(r_i) < 10^{-3} \nu$$

[i.e., a mean-square discrepancy $\sim 3\%$, between the numerical values of $W(r)$ and its fitting expression, was our limit of tolerance]. This detects $r$-intervals where equations (3.11) and (3.12) are both fulfilled. (2) When performing the second fit, the best-fit value of $\mathcal{R}_m$ is within $1 \sigma$ from the actual $\mathcal{R}_m$ value. Here also we test that the slope of $W$ is not too far from what is required. Such constraints should therefore select points where $\mathcal{R} < \min$ and (nearly) intersects $w$.

As outlined above, one might reasonably expect that a large fraction of clusters, at their boundaries, are far enough from sphericity that the expected system of maxima and minima, as well as their coincidences, is disrupted. The numerical noise in calculating $w$ is also quite large and can be expected to create severe problems. On the contrary, we found that all clusters with mass $M \gtrsim 4.2 \times 10^{14} h^{-1} M_\odot$ have at least one value of $r_m$ fulfilling the above requirements, while some clusters have 2 or 3 points where the fitting criteria are fulfilled. In the few cases, when the fitting criteria were satisfied at more than one $r_m$, we discarded $r_m$ values yielding $\Delta r$ outside an interval $0.3 A \sim 3 A$. This selection criterion left us with $\sim 97\%$ of the initial clusters. When more than one $r_m$ was still available, we selected the one corresponding to the smallest $\chi^2$; this last criterion was needed for $\sim 10\%$ of the clusters only.

Let us recall that the requirement of intersection between a minimum of $\mathcal{R}$ and a maximum of $w$ was found for spherical systems. When we deal with the halos of our simulations, sphericity is likely to be an approximation. When a single intersection exists, however, it is natural to guess that this is the point where the $R_w$ requirement is best approached. However, both in this case and when several $r_m$ points are found, it is natural to perform a closer inspection to make sure that no unexpected feature may bias our understanding of the physical situation.

This closer inspection requires an increased resolution. As described in §2, a TCDM model and a ΛCDM model were then reconsidered within a smaller box with sides of $180 h^{-1}$ Mpc, making use of the ART and GADGET codes. This gave us $\sim \frac{1}{3}$ of the clusters provided by the AP3M simulations but enabled us to focus on particular clusters, making use of the ART package facilities to increase the resolution there while still keeping identical boundary conditions. In order to test that the regularities found are not linked to peculiarities of the ART package, some clusters were magnified using GADGET instead of ART.
Altogether we have 12 clusters magnified, six for each model. Four of the latter were obtained using ART and three using GADGET; hence, one cluster was magnified with both codes, showing that our results are independent of the $N$-body code used. In fact, the final positions of particles have just minor differences, while $R$ and $W$ coincide. A number of subsequent tests also concerned the stability of the minima of $R$. In general, the number of local minima $r_m$ decreases when the resolution is increased, but the point where $W$ fits the equation (4.1) with the worst resolution is a minimum also with greater resolutions. In just a few cases, new minima arise when the resolution is improved; but in no case is a minimum yielding the BL erased when the resolution is changed. The “worst” cases for each model are shown in Figure 2. Here we have a TCDM cluster, taken from simulation C, which passes from three minima (128$^3$ particles), to one minimum (256$^3$ particles), and, again, to three minima (512$^3$ particles). The BL is displaced outward by $\sim 150 \, \h$ kpc when we pass from 128 to 256; then, when passing from 256 to 512, no appreciable shift occurs. Of the 12 clusters considered, only this one presents a shift slightly above the resolution of the initial simulation. The $\Lambda$CDM cluster of simulation D, shown in Figure 2, shows four minima with 128$^3$ particles, two minima with 256$^3$ particles, and, again, three minima with 512$^3$ particles; but when the resolution is changed, the shifts are smaller than $40 \, \h$ kpc.

For these 12 clusters we follow in detail the joint behavior of $R$ and $W$. We show them in Figure 3 for the best and worst cases we found. Of course, a precise coincidence between a minimum of $R$ and a maximum of $w$ would indicate that, within the resolution limits, the system is spherical. Seeking this kind of coincidence, therefore is somewhat fatuous. Furthermore, in order to work out $w$, we ought to differentiate $W$, which is obtained from a discrete point distribution. Hence, although the nice coincidence of the best case is quite appealing, this case is not safer than the worst case we show. By tolerating a $3\%$ disagreement in $W$, for $r/r_m \approx 1.1$, we allow for a tolerance $\sim 0.3$ in the exponent $w$. In the worst case, we find a $w$-$R$ discrepancy of this order, but in most cases, $|w-R|$ turns out to be $\sim 0.1$. We tentatively conclude that this resolution is sufficient to show physical features and that the level of the $w$-$R$ (dis)agreement is a measure of the $a$-sphericity of actual systems. The important issue is that we always find a maximum of $w$ to match the minimum of $R$, quite close to the $r_m$ selected at the initial resolution level.

This point can be further illustrated by Figure 4, which shows a plot similar to Figure 3 for a typical case at the initial resolution level. Both the $R$ and the $w$ curves are much noisier here. Curve $R$, in particular, shows a wide set of local minima; the only persistent minima, however, are those marked by thick filled circles. As expected, the behavior of $w$ is still noisier, and most of the oscillations shown are clearly numerical. The role of $w$, however, just amounts to choosing among the points marked by a thick filled circle and selecting the point marked by a vertical arrow. Even at
this resolution level, the presence of a maximum of \( w \), close to such point, can be suspected. When the resolution is increased, this maximum is more clearly visible, while no \( w \) maxima exist close to the other \( \Delta \) minima.

A further preliminary test of our technique, concerning galaxy-sized and unvirialized dark matter halos, is given in Appendix B.

Before concluding this section, let us draw the reader’s attention on the setting of the BL around particle agglomeration, as shown in Figure 5 for a CDM cluster. This figure shows that the BL is actually set outside of the main matter agglomeration; its spherical shape is somehow in contrast with the apparent \( a \)-sphericity of the cluster materials and easily justifies minor discrepancies from results based on an assumption of full spherical symmetry.

5. RESULTS

Once the sphere confining cluster materials is set, we can evaluate the density contrast \( \Delta \), and the mass \( M_c \), inside it. In Figures 6 and 7 points give \( \Delta \), and \( M_c \) for all clusters in simulations A and B, respectively. They show a rather wide spread of \( \Delta \) values. By subdividing the \( M_c \) abscessa in intervals of constant logarithmic width, we evaluate the average density contrast in each of them to seek systematic trends with mass. Averages are still subject to a significant uncertainty owing to the spread of \( \Delta \). They are shown, at the 1 \( \sigma \) level, in the plots. At high masses, some logarithmic intervals of Figure 7 are empty or contain a single object. In the latter cases no error bar is given.

There seems to be no evidence of any peculiar trend of density contrasts with mass apart from, perhaps, a modest indication of an increasing density contrast at very high mass contrasts we found; the average \( \Delta \), however, in both cases, is smaller than \( \Delta \), by \( \sim 25\% \).

It is, however, clear that gravitationally evolved, stationary objects are not uniquely identified with a given, fixed density contrast. In further work we plan to deal with the impact of variable \( \Delta \), on the physical characteristics of dark matter halos, such as concentration, average angular momentum, density, and velocity profiles. It may also be significant to test our results against the effects of different particle selection criteria, e.g., using the SKID algorithm instead of the SO one to preselect the dark matter halos.

In Figures 8 and 9 we plot \( r_c \) against \( M_c \), for simulations A and B, respectively. Here error bars account for the variance of \( r_c \) around its average, which is wider than the error of the average \( r_c \), shown in Figure 6. Solid and dotted curves show the expected behavior of \( r_c \) against \( M_c \), when the density contrast is set either at the average \( \Delta \) value or at \( \Delta \).

It is also significant to compare the plot of \( r_c \) against \( M_c \) with the behavior of the radii \( r_c \) against the masses \( M_c \) of the corresponding clusters. This comparison is shown in Figure 10, for simulation A only; in order to avoid confusion, we omit error bars, which, however, are approximately of the same size in both cases. The highest mass points, for which error bars cannot be evaluated, are also omitted. Filled circles yield \( r_c \) versus \( M_c \), empty circles yield \( r_c \) versus \( M_c \). Filled circles nicely fit the line worked out from the average density contrast \( \Delta \); only at high masses, where the statistics is poorer, are some of the circles far from this line. The same line is also a reasonable fit for the open circles. These, however, are systematically farther at all mass scales. In the figure, however, we also plot an horizontal line showing the average of the \( r_c \) values of all clusters with mass greater than \( 4.2 \times 10^{14} \, h^{-1} \, M_\odot \). Even this average can be considered a reasonable fit for open circles (an unweighted \( \chi^2 \) evaluation gives similar probabilities to both fitting lines). This plot shows that there are actual dangers, if quantities worked out assuming a constant \( \Delta \), are compared with real data. In this case, one might tentatively suggest that there is a typical, mass-independent, cluster radius \( R \approx 1.56 \, h^{-1} \, Mpc \) quite close to the Abell value. Our procedure, instead, outlines that this arises because some clusters were attributed a biased mass and the corresponding points were then set at a wrong abscissa. Although, altogether, this abscessa reshuffling is substantially casual, the danger that an characteristic scale erroneously appears is far from absent.

A critical result of our analysis is, however, shown in Figures 11 and 12 for simulations A and B, respectively. In simulations, the “numerical” cluster masses can be easily evaluated by summing up particle masses. The actual approach, in the real world, ought to be quite different and is based, first of all, on an analysis of galaxy velocities or X-ray–emitting gas temperature. These analysis make use of the virial hypothesis; therefore, measured masses of galaxy clusters are estimates of their dynamical masses. It is therefore important to test how “numerical” cluster masses in simulations agree with the masses

\[
M_{\text{dyn}} = \frac{\langle v^2 \rangle_{(r_c)} f_{(r_c)}}{G},
\]

evaluated averaging over the velocities of the particles within \( r_{c} \). This comparison has been often performed, showing a reasonable coincidence between \( M_c \) and \( M_{\text{dyn}} \). The results of such a fit are shown in Figures 11 and 12 by the dashed histograms, which confirm the slight excess of \( M_{\text{dyn}} \) versus \( M_c \) already noticed by previous authors. In the same plots we also show the results of a fit between \( M_{\text{dyn}} \)
and $M_c$, obtained on the basis of the setting of the BL. There seems to be little doubt that the latter fit is better. The average values of $M_{\text{dyn}}/M_c$ are both $0.97 \pm 0.03$, quite close to unity and consistent with it at the $1\sigma$ level.

We have also compared the shapes of the cluster (integral) mass functions $n_c(>M_c)$ and $n_i(>M_i)$. In Figures 13 and 14 upper and lower plots show their behaviors, respectively. In the same plots, we also show Press & Schechter and Sheth & Tormen theoretical curves. They can be obtained from two different expressions of

$$f(\nu)\nu d\log \nu = \frac{M}{\bar{\rho}_m} n_i(M) Md \log M ; \quad (5.2)$$

here $\bar{\rho}_m$ is matter density, the bias factor $\nu = \delta_c/\sigma_M$ is the ratio of the critical overdensity in the spherical growth model to the rms density fluctuation on the length scale corresponding to the mass $M$, and $n_i(M)$ is the differential mass function, which shall then be integrated to obtain $n_i(>M)$.

In the Press & Schechter formulation, assuming spherical unperturbed fluctuation growth,

$$f(\nu)\nu = \sqrt{2/\pi \nu} \exp(-\nu^2/2) , \quad (5.3)$$

while Sheth & Tormen, taking into account the ellipsoidal nature of the collapse, argue that

$$f(\nu)\nu = A(1 + \nu^{1-2q}) \sqrt{2/\pi \nu} \exp(-\nu^2/2) , \quad (5.4)$$

with $\nu = \sqrt{a} \nu$, an expression that introduces parameters $A$, $q$, and $a$, constrained, however, by the requirement that all matter is bound in objects of some mass $M$, however small, and that therefore the integral of $f(\nu)$ must be unity. In our plots, $A$ is normalized to yield the number of clusters found.

---

Fig. 5.—Image of a typical cluster, with the location of the BL. The cluster shown has a radius $r_c = 1.76 h^{-1}$ Mpc, a mass $M_c = 8.92 \times 10^{14} h^{-1} M_{\odot}$, and a density contrast $\Delta_c = 141$. The mean-square velocity of particles within $r_c$ is 1574 km s$^{-1}$. This cluster is taken from simulation D. Gray scales refer to particle velocities. [See the electronic edition of the Journal for a color version of this figure.]
in simulations, and this constraint is automatically satisfied. Sheth & Tormen (1999) showed that in the GIF simulations for an SCDM, ΩCDM, and ΛCDM models (see Kauffmann et al. 1999), a good fit to the numerical mass function was obtained if $\alpha = 0.3$, $\beta = 0.707$.

In Figures 13 and 14 we report the mass function obtained from equation (5.4) for these values, for TCDM and ΛCDM, respectively. The fit with the $n_c(M_c)$ is surely better than using equation (5.3). We also tried to modify parameter $\alpha$, which, according to Sheth & Tormen arguments, is related to the density contrast of virialized structures. As a matter of fact $n_c(M_c)$ is derived with a variable density contrast, as explained in previous sections, and, however, with an average final density contrast that is $\sim 25\%$ below $\Delta_c$. It is therefore reasonable to expect that a lower value of $\alpha$ is needed to compare theoretical predictions with the numerical behavior of $n_c(M_c)$. In Figures 13 and 14 we show the expression (5.4), for both $\alpha = 0.707$ and $\alpha = 0.5$. It is also evident that, while $\alpha = 0.707$ provides a good fit for $M_c$ mass functions, the fit obtained by $\alpha = 0.5$ for the $M_c$ mass function is perhaps better.
The results of these comparisons, altogether, are the following: (1) No major variations in the numerical mass function arise when $M_v$ is replaced by $M_c$. (2) Variations, however, exist, which are of the same order of the differences between the standard theoretical expression (eq. [5.3]; Press & Schechter) and the improved theoretical expression (eq. [5.4]; Sheth & Tormen). (3) When the latter expression is used, the fits to the numerical mass functions are best if different values of the parameter $a$ are used for $M_v$ and $M_c$ ($0.7$ and $0.5$, respectively). The differences between the mass functions $n_c(M_v)$ and $n_c(M_c)$ are more evident in the intermediate-mass range ($7 \times 10^{14} h^{-1} M_\odot < M < 10^{15} h^{-1} M_\odot$). They arise from a widespread "reshuffling" among the masses of dark matter halos, when the two definitions are used, causing thereby different numbers of halos in different mass intervals. This can also be seen from Figure 10, where the mean cluster radii ($r_c, r_v$) of halos in this mass range show appreciable differences.

Fig. 10.—We show how "virial" quantities can introduce spurious characteristic scales if fitted against "real" quantities. Here mean cluster radii ($r_v$) are plotted against $M_v$ (filled circles) and $M_c$ (open circles). Error bars are omitted to avoid confusion (see, however, Fig. 7). The horizontal line could be interpreted as a mass-independent average radius for all clusters. [See the electronic edition of the Journal for a color version of this figure.]

Fig. 11.—Ratio between masses evaluated from particle velocities, according to the virial theorem ($M_{dyn}$), and summing particle masses ($M_{cluster}$) is shown limiting clusters either at $r_c$ or at $r_v$, for all clusters of simulation A.

Fig. 12.—Same as Fig. 11, but for simulation B.

Fig. 13.—Comparison between mass functions obtained using BL or virial quantities (TCDM).
obtained under assumptions that can be incorrect in the real world as well as in simulations. Such assumptions, however, were explicitly considered to be the best possible choice. In particular, Cole & Lacey (1996) explored the possibility of using the virial ratio but considered its value in spheres instead of layers. Here we see that passing from the integral to the differential virial ratio, \( \mathcal{R}(r) = -2T(r)/W(r) \), allows the detection of a neat boundary, where a transition from halo to surrounding material occurs. In fact, first of all, (1) this inspection allows the detection of minimum points of \( \mathcal{R} \) in all halos, which could be easily missed in an integral inspection. Some of them are safely shown not to be numerical features, as they persist without appreciable shifts when we compare different resolution simulations of a given halo. Furthermore, (2) we found that quite close to the radius \( r \), where one of the persistent minima occurs, there is always a maximum of the function \( w(r) \). Finally, (3) at the radius \( r \), we also have

\[
w(r) \simeq \mathcal{R}(r) \quad .
\]

Let us recall that, in general, \( w(r) \) is defined with reference to the behavior of the potential energy around \( r \), by setting

\[
W(r) = W(\bar{r})(r/\bar{r})^{-w(r)} ,
\]

and, therefore, its \( r \) dependence accounts for the radial dependence of \( W(r) \).

In this paper we have shown that properties 1, 2, and 3 above are consistent with the following requirements: (a) the value \( r \) sets a neat boundary between bound and unbound material, and (b) a significant interval (depth \( \sim 50–100 \ h^{-1} \) kpc), where \( w(r) \) is constant, lies about \( r \). We called it a boundary layer. Accordingly, the \( r \) dependence of \( W(r) \), inside the BL, is expressed by equation (6.1), by replacing the exponent \( w(r) \) with its constant value \( w \).

The relation between the observed properties 1, 2, and 3 and requirements \( a \) and \( b \) was shown under the assumption of spherical symmetry. The fact that the properties 1, 2, and 3 are not satisfied exactly, but with a (slight) approximation, can easily be attributed to deviations of numerical structures from sphericity. However, such deviations ought to be quite mild, owing to the statistics we performed on a large number of halos, and this indicates that violent relaxation erased most previous \( a \)-spherical features. Nonspherical collapses, however, leave a substantial imprint on the final density contrasts, \( \Delta_n \), found for virialized halos whose spread accounts for different initial three-dimensional geometries of fluctuations and different interactions with the environment during the collapsing stages.

The simulations used to focus the above properties, at different levels of resolution, in TCDM and \( \Lambda \)CDM modes, were run with both the GADGET and the ART codes. Results do not depend on the code. We could also extend the analysis, at the lowest resolution level, to simulations run in quite large boxes (360 \( h^{-1} \) Mpc aside), where we had a large statistics of clusters (>300 with \( M_c > 4.2 \times 10^{14} \ h^{-1} M_\odot \) for each model). We applied to all of them an \( r_v \) requirement, meant to detect the BL, and found it in 97% of the clusters considered. A detailed inspection of these clusters shows that the mass \( M_\text{BL} \) within the BL substantially coincides with the mass \( M_\text{dy} \) evaluated from the velocities of all particles within \( r_v \), according to the virial theorem. Furthermore, a direct inspection of the clusters without a BL showed that they were exceptional structures, located where

![Fig. 14.—Comparison between mass functions obtained using BL or virial quantities (\( \Lambda \)CDM).](image-url)
a major merger is occurring, which certainly justified a dynamically unsettled condition and a badly $\alpha$-spherical geometry. Let us notice, however (see Fig. 5), that “standard” $\alpha$-sphericity of halo structures does not appear to be a serious obstacle to BL detection.

At present, model clusters to fit X-ray data are mostly built using hydro codes. This allows substantial improvements with respect to initial analyses based on pure Newtonian dynamics. There are, however, some features in the interpretation of both kinds of simulations, which rely on a sound definition of the virialization radius $R_v$. This radius, whose setting immediately follows from the detection of the BL position, corresponds to a wide spread of density contrasts $\Delta_v$, and, in general, is significantly different from the radius $R_c$, obtained using a given density contrast $\Delta_c$. Even keeping to models without hydrodynamics, it is clear that using different radii $R_v$ and density contrast $\Delta_v$ could lead to different relations among $L_X$, $T_X$, and $M_c$. As a consequence, the one-to-one correspondence between $M_c$ and $T_X$ could be lost and it would no longer be granted that a mass function and a temperature function are substantially equivalent quantities.

We thank INAF for allowing us the CPU time to perform ART simulations C and D at the CINECA consortium (grant cnami44a on the SGI Origin 3800 machine). GADGET simulations of high-resolution clusters have been run on the 16 Linux PC Beowulf cluster at the Osservatorio Astronomico di Torino. A. Gardini is thanked for allowing us to make use of simulations A and B; we also wish to thank him, Loris Colombo, and Giuseppe Tormen for useful discussions during the preparation of this paper.

APPENDIX A

Let us assume that halos are spherically symmetric. If BLs are in virial equilibrium, at any $r$, in their interior

$$M(<r)$$

being the mass inside $r$. According to kinetic gas theory, however, $p = \rho<v^2>/3$. Accordingly, local equilibrium prescribes that $p = -\rho\dot{v}/3$ and, up to first order in $\Delta r/r$,

$$3(p_+V_+ - p_-V_-) = \frac{4\pi}{3} G \rho_+ r^3 - \beta \left( \frac{M_+}{r^3} - \frac{M_-}{r^3} \right)$$

$$\approx \frac{4\pi}{3} G \rho_+ r^3 \left( \frac{2\beta - 1}{3} M_- \Delta r \right)$$

with a $\beta$ value such that $\rho r^{3-\beta}$ is constant across $\Delta r$ (the indices + and − indicate that a quantity is evaluated in $r_\pm$).

Let us compare this term with the potential energy of the layer

$$W = G \int_{r_\pm}^{r} d^3 r \rho(r) \frac{M(<r)}{r} \approx \frac{4\pi}{3} G \rho_+ r^3 \left( \frac{M_- \Delta r}{r_\pm - r_-} \right)$$

also evaluated assuming spherical symmetry and neglecting terms of higher order in $\Delta r/r$. The ratio between $pV$ terms and potential energy is $\approx(2\beta - 1)/3$ and would vanish for $\beta = 0.5$.

Let us now assume halos whose profile is $\rho(r) \approx \rho_0 \chi(r/r_0)$ with

$$\chi(x) = \left[x^{A}(1 + x)^{3-A}\right]^{-1}$$

where $r_0$ is the scale radius of the profile and the concentration of the halo is $c = r_0/r_c$. This profile is found for most halos in our simulations, up to $r < r_c$, with a value of $\alpha$ in the interval 4–7 and values of $\alpha \approx 1$; this agrees with previous numerical analyses (see, e.g., Navarro et al. 1996, 1997; Ghigna et al. 2000; Klypin et al. 2001; Power et al. 2002), also extended to smaller values of $r$, finding values of $\alpha$ ranging between 0.8 and 1.2. Using this profile we can evaluate the $r$ dependence of $\beta$ for $\alpha$ values in the above interval. Such values are shown in Figure 15 and indicate that for $c \approx 4-7, \beta \sim 0.5-0.3$.

This shows that the contribution of the pressure terms to the virial balance is expected to be significantly smaller than the contribution of the potential term.

Let us, however, add some further comments:

1. Using the profile in equation (A4) for $r > r_c$ is an approximation. An inspection of numerical halos, already significantly inhomogeneous at such radii (see, e.g., Fig. 5), shows that the slope of the profile is often smoother there.

2. Accordingly, owing to equations (A2) and (A3), the $pV$ terms can be absorbed in a factor ($\sim 1$), set in front of the potential term of the virial balance. This correction does not cause any displacement of the point at which $\beta$ has its minimum. On the contrary, it may interfere with the condition $w = \beta$, which, in principle, can be suitably improved.

3. Deviations from spherical symmetry, however, are far from being fully negligible, and the discrepancies between $\beta$ and $w$, found in halo analysis, show that a correction of $\beta$ by $\sim 10\%$, would not improve the efficiency of the method.
APPENDIX B

We tried to find a BL, i.e., to apply the $R_w$ requirement, also in two $N$-body simulations aimed at studying the evolution of a galactic stellar disk in a cosmological context. These simulations, performed with GADGET, will be discussed in a forthcoming paper (A. Murante, G. Curir, & P. Mazzei 2003, in preparation). Here we used simulations with dark matter only (no galactic disk is present).

In the first one, initial conditions were set up with the same multimass technique described in § 2, using the ART package. A dark matter halo, whose mass is $M_v = 1.14 \times 10^{11} h^{-1} M_\odot$, at redshift $z = 0$, was simulated at high resolution using dark matter particles of mass $M_p = 1.21 \times 10^6 h^{-1} M_\odot$. According to equation (1.1), the virial radius $r_v = 0.125 h^{-1}$ Mpc. External forces were taken into account by setting heavier and heavier particles in three concentric shells. We checked that no intruders (heavier mass particles) were ever closer than $0.5 h^{-1}$ Mpc from the center of mass of the halo. The $R_w$ requirement was applied to this halo, at redshifts $z = 0$ and $z = 2$.

At $z = 0$ a BL was found, with a radius $r_c = 0.113 h^{-1}$ Mpc, yielding a ratio $M_c/M_{\text{dyn}} = 1.0502$. On the contrary, at $z = 2$, we could not find a good fit for the $\chi^2$ parameter used to implement the $R_w$ requirement. It should be noticed that these results held, in spite of the fact that the halo concentration is ≈20.

This also suggests that BLs are found by the $R_w$ requirement when the condition $pr^3 = \text{const}$ is (mildly) violated; on the contrary, no BL is found when the halo is not yet virialized, as it was at $z = 2$ and is also confirmed by direct inspection. Apparently, the presence of a BL, however, distinguishes gravitationally relaxed objects from those still in an evolutionary phase.

A partial confirm of these two results comes from the application of the $R_w$ requirement to a second simulation, following the evolution of an isolated halo of nominal mass equal to the previous one, with a nominal radius of $R = 0.180$ Mpc, generated with a NFW density profile (see eq. [A4]) and with initial particle velocities picked up from a multivariate Maxwellian distribution; the NFW density profile was cut off at the nominal radius; the concentration $c$ was set to the value measured in the previous case (using $r_v$ to evaluate it, as in Navarro et al. 1997). The halo was evolved for $\approx 10$ Gyr, to reach the age of the universe at $z = 2$ in a $\Lambda$CDM cosmology where $\Omega_\Lambda = 0.7$ and $\Omega_m = 0.3$.

We applied the $R_w$ algorithm, to find a BL at the beginning ($t = 0$ Gyr) and at the end ($t = 10.23$ Gyr) of the simulation. No BL could be found at $t = 0$, when the halo was not in equilibrium. Apparently, therefore, the presence of a BL is characteristic of gravitationally stable objects, independently of the geometrical distribution of particles. At $t = 0$, a SO algorithm, based on a purely geometrical prescription, would comfortably detect a halo. The $R_w$ requirement, instead, which is based on dynamical prescriptions, appears to be more selective than purely geometrical recipes.

At $t = 10.23$ Gyr, we find a layer fulfilling the $R_w$ requirement, with $r_c = 0.023$ Mpc, yielding $M_c/M_{\text{dyn}} = 1.0201$. This happens in spite of the value of the density contrast at $r_c$, which is quite large ($\rho/\rho_{\text{crit}} = 2457$). In this (quite peculiar) case, the definition of virialization based on the density contrast fails, in spite of the fact that gravitational equilibrium is established.

Fig. 15.—$\beta$ yields the deviation from three of the slopes of the halo profile in the region where the BL is expected to lie.
These arguments seem to indicate that a technique based on the $R_w$ requirement is applicable on a wide range of dark matter halo masses, even when $c$ is fairly large; mild deviations from the requirement that $pr^3$ is constant do not seem to destroy its effectiveness. Further analysis will be performed to put precise limits to the cases when the $R_w$ criterion is a useful tool for telling apart virialized halos from still strongly evolving ones.

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