Shock finding on a moving-mesh: I. Shock statistics in non-radiative cosmological simulations

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ABSTRACT
Cosmological shock waves play an important role in hierarchical structure formation by dissipating and thermalizing kinetic energy of gas flows, thereby heating the universe. Furthermore, identifying shocks in hydrodynamical simulations and measuring their Mach number accurately is critical for calculating the production of non-thermal particle components through diffusive shock acceleration. However, shocks are often significantly broadened in numerical simulations, making it challenging to implement an accurate shock finder. We here introduce a refined methodology for detecting shocks in the moving-mesh code AREPO, and show that results for shock statistics can be sensitive to implementation details. We put special emphasis on filtering against spurious shock detections due to tangential discontinuities and contacts. Both of them are omnipresent in cosmological simulations, for example in the form of shear-induced Kelvin-Helmholtz instabilities and cold fronts. As an initial application of our new implementation, we analyse shock statistics in non-radiative cosmological simulations of dark matter and baryons. We find that the bulk of energy dissipation at redshift zero occurs in shocks with Mach numbers around $M \approx 2.7$. Furthermore, almost 40\% of the thermalization is contributed by shocks in the warm hot intergalactic medium (WHIM), whereas $\approx 60\%$ occurs in clusters, groups and smaller halos. Compared to previous studies, these findings revise the characterization of the most important shocks towards higher Mach numbers and lower density structures. Our results also suggest that regions with densities above and below $\delta_b = 100$ should be roughly equally important for the energetics of cosmic ray acceleration through large-scale structure shocks.

Key words: large-scale structure of Universe – galaxies: clusters: general – hydrodynamics – shock waves – methods: numerical

1 INTRODUCTION

The collapse of dark and baryonic matter during hierarchical large-scale structure formation releases gravitational energy and transforms it into kinetic energy. The bulk of the kinetic energy of the gas gets dissipated by cosmological shocks, heating the gas in virialized halos (for example the intracluster medium, ICM) as well as in the warm-hot intergalactic medium (WHIM). Cosmological hydrodynamic shocks are collisionless; they are established due to plasma interactions by means of magnetic fields. They can themselves amplify magnetic fields and accelerate particles via diffusive shock acceleration (DSA; Blandford & Ostriker 1978; Malkov & O’C Drury 2001) up to relativistic energies, producing cosmic rays.

Directly observing cosmological shocks is challenging, especially outside cluster cores where the X-ray emission is weak. An obvious approach is to look for jumps in the thermal gas quantities. In this way, and using exquisite X-ray data from the Chandra telescope, the first merger shocks have been confirmed in the bullet cluster (Markevitch et al. 2002; Markevitch 2006, $M \approx 3$) and in the train-wreck cluster (Markevitch et al. 2005, $M \approx 2.1$). Maps of the gas density and the temperature can be inferred from the luminosity and the spectrum of the X-ray radiation, respectively. Both are necessary in order to calculate a pressure map and confirm a shock. Furthermore, it is possible to directly measure a pressure jump by means of the thermal Sunyaev-Zel’dovich signal. For example, steep pressure gradients have been detected inside $R_{500}$ in the nearby Coma cluster (Planck Collaboration et al. 2013). The location of the gradients coincides with temperature jumps, and two shocks with Mach numbers around $M \approx 2$ were reported in this way.

Shocks can also be observed indirectly at radio wavelengths. Diffusively shock-accelerated cosmic ray electrons in merger and accretion shocks produce synchrotron radiation, so-called radio gischt (Ensslin et al. 1998; Battaglia et al. 2009; Pinzke et al. 2013). This phenomenon has been observed in several clusters (see for example Clarke & Ensslin 2006; Bonafede et al. 2009; van Weeren...
Cosmological shocks in numerical simulations of large-scale structure formation were analysed comprehensively in previous studies, for example in Quilis et al. (1998), Miniati et al. (2000), Ryu et al. (2003), Pfrommer et al. (2006), Kang et al. (2007), Skillman et al. (2008), Vazza et al. (2009), Planelles & Quilis (2013), and Hong et al. (2014). The detected shocks can be divided into two distinct classes, external and internal shocks (Ryu et al. 2003). Strong external shocks form when previously cold and unshocked gas ($T \lesssim 10^4$) accretes from voids onto the cosmic web. They have typically high Mach numbers up to $M \approx 100$, but dissipate comparatively little energy due to the low preshock density and temperature. Internal shocks on the other hand occur if previously shocked and thus hotter gas inside non-linear structures gets shock-heated further. Because of the smaller temperature ratios compared to external shocks, the Mach numbers of internal shocks are typically smaller ($M \lesssim 10$). The preshock density and temperature of internal shocks is however high. This allows them to account for the bulk of the energy dissipation, especially shocks with Mach numbers in the range $2 \lesssim M \lesssim 4$ contribute strongly.

A detailed characterization of the prevalence and strength of shocks in numerical simulations requires the implementation of an accurate shock finder. The first approaches in grid-based cosmological codes simply used the jump conditions on a cell-by-cell basis to identify shocked cells (Quilis et al. 1998; Miniati et al. 2000). As a first improvement, Ryu et al. (2003) proposed a method in which the shock centres are identified in a two step procedure. First, cells are considered to be in a shock zone if they simultaneously meet three different criteria meant to identify cells with some numerical shock dissipation. Within this zone, the shock centres were then determined by looking for the cells with the maximum compression. This more elaborate approach takes into account that the common numerical methods capture a shock discontinuity over a few cells, rather than exposing the full jump strength at a single cell interface.

In order to deal with three dimensional simulations, Ryu et al. (2003) calculated three different Mach numbers ($M_x$, $M_y$, $M_z$) for each cell in the shock centre by evaluating the temperature jump across the shock zone in each coordinate direction. The maximum occurring Mach number was then assigned to the shock cell. A refinement to this method is to calculate the Mach number via the pre- and postshock temperature and density. The result of the shock finder becomes independent of the orientation between the shock and the underlying grid. The shock-finding implementation of Skillman et al. (2008) additionally filters tangential discontinuities and contacts by evaluating the pre- and postshock temperature and density.

Quite different shock detection methodologies have been developed for Lagrangian smoothed-particle hydrodynamics (SPH) codes. To this end, Keshet et al. (2003) measured the entropy increase of each particle between different snapshots, and Pfrommer et al. (2006) measured the entropy injection rate on a per-particle basis during the simulation. As the entropy production is directly sourced by the artificial viscosity used for shock capturing in SPH, this allows an estimate of the Mach number of a shock. In another SPH shock-finding method, Hoteit et al. (2008) proposed to use the local entropy gradient for determining associated pre- and post-shock regions, and then to calculate the Mach number across the associated jump.

In a recent code comparison project, Vazza et al. (2011) reported reasonable agreement of different codes with respect to energy dissipation and shock abundance as a function of Mach number. However, significant differences have also been detected. Especially the detailed comparison of grid-based shock finders with the SPH-based techniques revealed some apparent inconsistencies in the shock morphologies and in various features in the gas phase-space diagrams. These discrepancies in the results of the different shock finder implementations highlight the computational challenges involved in accurate numerical shock detection. As we will demonstrate in this work, a shock finder can be very sensitive to implementation details, and it is hence crucial to improve these methods further, for example by more carefully removing false positive shock detections associated with tangential and contact discontinuities.

This is the goal of this paper, which has the following structure. We describe and validate our new methodology for finding shocks in the moving-mesh code AREPO in Sections 2 and 3, respectively. The shock finder is then applied to non-radiative simulations in Section 4, and differences to previous studies are discussed in Section 5. Finally, we summarise our results in Section 6.

2 METHODOLOGY

2.1 The moving-mesh code AREPO

The non-radiative cosmological simulations analysed in this paper as well as the development of the shock detection method were carried out using the AREPO code (Springel 2010). In this cosmological hydrodynamical code, the gas physics is calculated on a moving Voronoi mesh. The mesh generating points are advected with the local velocity of the fluid in order to achieve quasi-Lagrangian behaviour. For solving the Euler equations on the unstructured Voronoi grid, a finite volume method is used in the form of a second-order unsplit Godunov scheme with an exact Riemann solver. With this approach the accuracy of a grid code can be combined with features of Lagrangian codes such as Galilean-invariance and approximately constant mass per resolution element. Gravity exerted by the gas and the dark matter is computed with a Tree-PM method (Xu 1995; Springel 2005) in which long-range gravitational forces are calculated with a particle-mesh scheme, whereas short-range interactions are calculated in real space using a hierarchical multipole expansion organized with an octree (Barnes & Hut 1986).

2.2 The Rankine-Hugoniot Jump Conditions

It is well known that the mass, momentum and energy flux is continuous across a discontinuity in an ideal gas. If the mass flux happens to be zero, it follows that the normal component of the velocity and the pressure do not jump across the discontinuity (‘tangential
discontinuities’). If additionally the tangential velocity is also continuous, a special discontinuity is present which is called a contact. A non-zero mass flux on the other hand implies that the tangential velocities are continuous. In this case, a shock is present and the normal velocities as well as the other thermodynamic variables jump according to (Landau & Lifshitz 1966)

\[
\frac{p_2}{p_1} = \frac{v_1}{v_2} = \frac{(y + 1)M^2}{(y - 1)M^2 + 2},
\]

(1)

\[
\frac{p_2}{p_1} = \frac{2yM^2}{y + 1} - \frac{y - 1}{y + 1},
\]

(2)

\[
\frac{T_2}{T_1} = \frac{2(yM^2 - (y - 1)[(y - 1)M^2 + 2])}{(y + 1)^2M^2},
\]

(3)

\[
\frac{S_2}{S_1} = \left(\frac{2yM^2}{y + 1} - \frac{y - 1}{y + 1}\right)\left(\frac{(y - 1)M^2 + 2}{(y + 1)^2M^2}\right)^\gamma.
\]

(4)

The quantities \(p, p, T, S = p/p\) denote density, pressure, temperature, and the entropic function, respectively. \(M\) is the Mach number of the shock, \(x\) the adiabatic index of the gas, and the indices 1 and 2 label the preshock and postshock regions, respectively.

### 2.3 Shock-finding Method for AREPO

We base the implementation of our shock finder on a number of previous ideas (Ryu et al. 2003; Skillman et al. 2008; Hong et al. 2014), augmented with some improvements. First of all, a shock zone is identified by appropriate criteria which put special emphasis on filtering spurious shocks such as tangential discontinuities and contacts. Note that this part of criterion (iii) on its own may not be sufficient since gravitationally compressed cells are also able to fulfill it. \(\Delta \log T\) and \(\Delta \log p\) are calculated with the temperature and pressure of neighbouring cells along the shock direction. The logarithm is taken such that the calculation can be accomplished with a difference in order to avoid inaccurate divisions in low temperature and pressure regimes. In our analysis, the minimum Mach number is set to \(M_{\text{min}} = 1.3\). We want to remark that the third criterion also rules out shocks with a slightly higher Mach number, since it is a local lower limit and the shock is broadened over a few cells. Note that we show in Section 3.2 that already \(M = 1.5\) shocks are fully captured.

In the following, we refer to the cells directly outside the shock zone in the direction of the positive temperature gradient as post-shock region, while the corresponding cells in the direction of the negative temperature gradient are referred to as preshock region.

#### 2.3.1 Shock Direction

For our method, the direction of shock propagation in each Voronoi cell has to be specified. In order to be consistent with the Mach number calculation (see Section 2.3.4), we use the unlimited temperature gradient for calculating the shock direction:

\[
d_s = \frac{-\nabla T}{|\nabla T|},
\]

(5)

where \(\nabla T\) is computed with the second-order accurate gradient operator available in AREPO for Voronoi meshes.

#### 2.3.2 Shock Zone

The first part of our algorithm consists of a loop over all cells. A cell is flagged as being in the shock zone, if the following criteria are met:

(i) \(\nabla v < 0\),

(ii) \(\nabla T \cdot \nabla p > 0\),

(iii) \(\Delta \log T \geq \log \frac{T_2}{T_1}\big|_{M=M_{\text{min}}} \quad \Delta \log p \geq \log \frac{p_2}{p_1}\big|_{M=M_{\text{min}}}\).

The first criterion is the standard compression criterion for shocks; whenever a shock is present, this condition is true. It also in principle filters tangential and contact discontinuities, however, this is not effective in real-world numerical simulations.

The second criterion is constructed such that spurious shock detections, potentially in a shear-flow or a cold front, are filtered out. Constant pressure implies that the density is inversely proportional to temperature and therefore these variables increase in opposite directions. At the same time, criterion (ii) holds in shocked cells.

The third criterion is a numerical guard against detecting spurious weak shocks. The first part of this protection mechanism introduces a lower boundary for the temperature jump, as in Ryu et al. (2003). The second part demands a minimum pressure jump, which again discriminates against tangential discontinuities and contacts. The third part of this protection mechanism introduces a lower boundary for the pressure jump, as in Ryu et al. (2003). The second part demands a minimum pressure jump, which again discriminates against tangential discontinuities and contacts. The third part of this protection mechanism introduces a lower boundary for the pressure jump, as in Ryu et al. (2003). The second part demands a minimum pressure jump, which again discriminates against tangential discontinuities and contacts. The third part of this protection mechanism introduces a lower boundary for the pressure jump, as in Ryu et al. (2003). The second part demands a minimum pressure jump, which again discriminates against tangential discontinuities and contacts.

#### 2.3.3 Shock Surface

After the determination of the shock zone, which has a typical thickness of 3-4 cells, we proceed with the construction of a shock surface consisting of a single layer of cells. For this purpose, rays are sent from each cell of the shock zone in the direction of the postshock region (along the temperature gradient). When the first cell outside of the shock zone is reached, the postshock temperature is recorded and the ray direction is reversed in order to find the preshock region. Furthermore, each ray stores the divergence of the cell from which it started. If a ray traverses a cell with a smaller divergence, the ray is discarded. For the rays reaching the preshock region, the Mach number is calculated via the temperature jump of eqn. (3) and assigned to the original cell of the ray. We call these cells with minimum divergence (i.e. maximum compression) across the shock zone the shock surface cells. In this way, a Mach number is only calculated for cells in the shock surface. In the rare case that the direction of the temperature jump inferred from the pre- and postshock temperatures is not consistent with the shock direction (given by the temperature gradient in the shocked cell), the detected feature is discarded.

In order to correctly treat overlapping shock zones of shocks propagating in opposite directions, we calculate in each step along a ray the scalar product of the shock direction of the original cell with the shock direction of the current cell. If the product is negative, the current temperature is recorded and the ray turns around or stops, depending on whether it was heading for the pre- or postshock region, respectively. With this approach we ensure that even when the shock zones of two different shocks overlap we are usually able to distinguish them and calculate their correct Mach numbers.

For the sake of bookkeeping simplicity in the distributed memory parallelization of the algorithm, we send only one ray per shock zone cell combined with reverting its direction once, instead of simultaneously sending two separate rays in opposite directions. Since the shock surface is very close to the postshock region (see
2.3.4 Mach Number Calculation

Given the pre- and postshock values, the Mach number can in principle be calculated with any of the equations (1) to (4). Note however that the Mach number calculation with the entropy jump has to be accomplished with a numerical root finder, for example a Newton-Raphson method. In Section 3.2 below, we investigate the quality of the practical results achieved with each of these Mach number determination methods and conclude that the temperature jump is best suited for the computation of the Mach number in AREPO, see also Fig. 2.

2.4 Energy Dissipation

The thermal energy created at a shock can be expressed in terms of a generated thermal energy flux (Ryu et al. 2003):

\[ f_{th} = \left| e_2 - e_1 \left( \frac{\rho_2}{\rho_1} \right)^{\gamma} \right| v_2. \]

(6)

The indices 1 and 2 indicate the pre- and postshock quantities, respectively, and \( e \) denotes the thermal energy per unit volume. This flux can be expressed as a fraction of the incoming kinetic energy flux \( f_k = \frac{1}{2} \rho_1 c_s M^2 \) :

\[ f_{th} = \delta(M) f_k. \]

(7)

The thermalization efficiency \( \delta(M) \) can be calculated from the Rankine-Hugoniot jump conditions (Kang et al. 2007), yielding

\[ \delta(M) = \frac{2}{\gamma(\gamma - 1) M R} \left[ 2 \frac{\gamma M^2}{\gamma + 1} - (\gamma - 1) R^2 \right], \]

(8)

where \( R \) represents the density jump:

\[ R \equiv \frac{\rho_2}{\rho_1} = \frac{(\gamma + 1) M^2}{(\gamma - 1) M^2 + 2}. \]

(9)

In our analysis, we use equation (7) for calculating the generated thermal energy flux of a cell in the shock surface. Given the area of the shock surface within a shocked cell (see Section 3.1), we are then also able to calculate the total dissipated energy per unit time.

3 VALIDATION

3.1 Sedov-Taylor Blast Wave

We test the determination of the shock surface with simulations of three-dimensional point explosions. We performed runs with 50³ and 100³ cells. In order to obtain an unstructured Voronoi mesh free of any preferred directions for the initial conditions, we distribute mesh-generating particles randomly in the unit box \( (x, y, z) \in [0, 1]^3 \). The mesh is then relaxed via Lloyd’s algorithm (Lloyd 1982) such that a glass-like configuration is obtained. We then set up the initial conditions as follows: The whole box is filled with uniform gas of density \( \rho_1 = 1 \) and pressure \( p \approx 10^{-4} \); the initial velocities are zero, and the adiabatic index is set to \( \gamma = 5/3 \). The energy \( E = 1 \) is injected into a single central cell of the grid.

We show a cross section of the 50³ simulation at \( t = 0.08 \) in the top panel of Figure 1. At the corners of the box the initial glass-like grid is still visible. Note however that the cross section of a three-dimensional Voronoi grid is in general no longer a Voronoi tesselation itself. The colour of the cells represents the density field of the fluid. The cells inside the white contours constitute the identified shock zone. The shock surface consists of the cells inside the black contour lines and features a position that agrees well with the expected position (extent of the green cross).

Determining the correct shock surface area is important for calculating the energy dissipation accurately. We describe in Section 3.2 how we measure this area from the shock surface cells. In the bottom panel of Fig. 1 we compare the time evolution of the measured surface area of the Sedov shock sphere with the analytic...
solution, which is given by $S(t) = 4\pi R^2(t)$ (green line), where $R(t) = \beta(E t / p_1)^{1/3}$ (Landau & Lifshitz 1966). The coefficient $\beta$ can be calculated numerically. We obtain the value $\beta = 1.152$ for $\gamma = 5/3$ from the code provided in Kamm & Timmes (2007). Our measurement tracks the expected scaling well but shows a small systematic overestimation of ~5%. We suspect the primary cause of the offset does not lie in the shock surface estimation itself but rather appears because the simulated blast wave is slightly ahead of the analytic solution due to low resolution present at early times (Springel 2010) in this self-similar problem.

3.2 Shock Tubes

We also checked the accuracy of the Mach number estimate for the identified shock surface by performing numerous shock tube tests (Sod 1978). In view of our target applications, we chose to adopt a three-dimensional box $(x, y, z) \in [0, 100] \times [0, 20] \times [0, 20]$ in all the tests. Again, a hydrodynamic glass-like initial grid is used with $4 \times 10^3$ cells. The gas has an adiabatic index of $\gamma = 5/3$, and the initial position of the discontinuity is prepared at $x = 50$. The variables of the right state $(x > 50)$ are set to $p_2 = 0.1$, $\rho_2 = 0.125$, and $v_z = 0$. The density and the velocity of the left state $(x < 50)$ are $\rho_1$ and $v_z = 0$, respectively. Furthermore, we assign a pressure $p_1$ to the left state such that the shock has a specific Mach number, see Table 1. The third column of the table shows the simulation time at which the shock reaches $x = 75$. We apply our shock finder to the corresponding output file. Note that the shock finder in this test, in contrast to the Sedov-Taylor blast wave, is also confronted with rarefaction waves and contact discontinuities, which obviously should not be mistaken as shock features by the shock finder.

The left panel of Figure 2 shows the quality of the Mach number determination for all considered Mach number calculation methods according to equations (1) to (4), except for the density jump method which is omitted because it is not sensitive for high Mach numbers because $\rho_2/p_1 \rightarrow (\gamma + 1)/(\gamma - 1)$ for $M \rightarrow \infty$. We note that in order to apply the velocity jump method, the velocities have to be transformed into the lab frame (Vazza et al. 2009).

The overall best results with AREPO for the shock tube tests are obtained with the temperature jump method according to equation (3). It performs very well for Mach numbers $M \geq 2$, as can be seen in the middle panel of Figure 2. For small Mach numbers ($M < 2$), there are mild postshock oscillations which cause the temperature jump method to underestimate the Mach number by a few percent. This systematic offset is present for all jump methods, unless the entropy jump is used, which is not perturbed by these adiabatic oscillations.

For calculating the energy dissipation, the correct shock surface area has to be determined. The area contribution $S_i$ of a single cell to the whole shock surface is expected to scale with its volume according to $V_i^{2/3}$. Furthermore, $S_i$ also depends on the shape of the cell. Cells in a shock are compressed normal to the shock direction and the degree of the compression depends on the strength of the shock. We therefore make the ansatz $S_i = \alpha F_i^{\beta} V_i^{2/3}$, where $F_i$ is the maximum face angle of the Voronoi cell, which characterizes the shape of the cell. The definition of this quantity has been

![Figure 2](image_url)

**Figure 2.** Left panel: Number of shock surface cells $N$ per Mach number bin for ten different shock tube tests (see Table 1) for different calculation methods of the Mach number. We obtain the best results for the temperature jump of equation (3). Middle panel: Mach number distributions of single shock tubes obtained with the temperature jump method. Low Mach numbers such as $M = 1.5$ are slightly underestimated due to mild postshock oscillations. This effect vanishes for Mach numbers $M \geq 2$, where the correct value is found with an accuracy of one percent. In both the left and middle panels, each histogram is normalized such that the area under the curve is unity. Right panel: Thermal energy fluxes in shock tubes, separately for the adiabatic and dissipative components. We compare the measurement using the temperature jump with the analytic solution, finding excellent agreement.

| $p_1$    | $M$    | $t_{end}$ |
|----------|--------|-----------|
| 0.8145190 | 1.5    | 14.43     |
| 1.9083018 | 2.0    | 10.83     |
| 15.357679 | 5.0    | 4.330     |
| 63.498622 | 10.0   | 2.165     |
| 400.51500 | 25.0   | 0.8660    |
| 1604.1492 | 50.0   | 0.4330    |
| 6418.6865 | 100.0  | 0.2165    |
| 40120.448 | 250.0  | 0.08660   |
| 160483.88 | 500.0  | 0.04330   |
| 641937.62 | 1000.0 | 0.02165   |

**Table 1.** Shock tube initial conditions. The pressure of the left state ($p_1$) is varied such that the shock has a specific Mach number. The right column indicates the time $t_{end}$ when the shock has traversed three quarters of the tube, at which point we measure its strength with our shock finder implementation.
4 SHOCKS IN NON-RADIATIVE SIMULATIONS

4.1 Simulation Setup

Besides full physics runs, the Illustris simulation suite (Vogelsberger et al. 2014a,b; Genel et al. 2014) contains also dark matter only as well as non-radiative runs. In this work we investigate shocks in the non-radiative runs, which include dark matter as well as gas, but no radiative cooling, star formation, and feedback. The cosmological parameters are consistent with the nine-year Wilkinson Microwave Anisotropy Probe (WMAP 9) measurements (Hinshaw et al. 2013), and are given by: \( \Omega_m = 0.2726 \), \( \Omega_b = 0.7274 \), \( \Omega_k = 0.0456 \), \( \sigma_8 = 0.809 \), \( n_s = 0.963 \) and \( H_0 = 100 \, h \, \text{km s}^{-1} \text{Mpc}^{-1} \) with \( h = 0.704 \). Two simulations with a resolution of \( 2 \times 455^3 \) and \( 2 \times 910^3 \) were carried out in a periodic box having \( 75 \, h^{-1} \text{Mpc} \) on a side. In the following, we refer to these runs as Illustris-NR-3 and Illustris-NR-2, where the latter is the one with the higher resolution.

4.2 Shock Finder Assessment

First of all, we use the non-radiative runs for assessing the overall quality of our shock finder. To this end, we compare the total dissipated energy per unit time obtained with the shock finder with the dissipated energy measured between two consecutive time-steps of the simulation. Under the assumption that the thermal energy during one time-step changes only due to dissipation and adiabatic compression and expansion, we can write for every cell:

\[
\frac{\Delta E_{\text{diss}}}{\Delta t} = \rho u_1 \left[ \frac{\gamma}{\gamma - 1} \right]^{\gamma - 1} m_1.
\]

Here \( \rho \) denotes the thermal energy per unit mass, \( m \) the mass, \( \rho \) the physical density, and the indices 1 and 2 correspond to quantities before and after the time-step, respectively. We divide equation (10) by the time-step size times the comoving box volume and solve for \( F_{\text{th, simulation}} = \Delta E_{\text{diss}} / (\Delta V) \), the dissipated energy per time and volume.

The comparison with the shock finder measurement is shown in the top panel of Figure 3. We find that our shock finder recovers the full amount of dissipated energy for low redshifts within 15\% accuracy. For very high redshifts, a progressively larger deviation occurs and our shock detection results do not account for all the dissipated energy any more. The origin of this difference lies in the topology of early shocks, which are not yet pronounced and resolved well at high redshift. Instead, they are rather scattered and occupy a large fraction of the simulation volume. As can be seen in the bottom panel of Figure 3, the deviation kicks in at progressively higher redshift for higher resolution simulations. We hence conclude that our shock finder statistics has an effective redshift completeness limit which depends on the resolution. We can trust the shock detection results from \( z = 0 \) up to \( z \approx 4.0 \) or \( z \approx 5.0 \) for the Illustris-NR-3 or Illustris-NR-2 runs, respectively.

4.3 Reionization Modelling

The simulations Illustris-NR-3 and Illustris-NR-2 have no significant temperature floor and do not model cosmic reionization during their runtime. However, it is important to account for the nearly uniform heating of the ambient gas at the reionization redshift (\( z \approx 6 \sim 7 \)) in order to avoid overestimating the Mach numbers of shocks from voids onto filaments at late times. For this purpose, we use a temperature floor of \( 10^4 \text{K} \) for the shock finding carried
Shock statistics in non-radiative moving-mesh simulations

Figure 4. Top panel: Projections of the temperature and baryonic over density of the Illustris-NR-2 run at redshift $z = 0$. The width and the height of the plots correspond to the full box size ($75 h^{-1}$Mpc). The projection in the $z$-direction has a depth of 150 kpc and is centred onto the biggest halo in the simulation. Bottom panel: Mach number field and energy dissipation rate density for the top left quarter of the box. Strong external shocks with Mach numbers up to $M \sim 100$ onto the super-cluster are visible, as well as mostly weak shocks in the interior. However, most of the energy gets dissipated internally due to the higher preshock density and temperature. Note that we do not find many shocks inside the accretion shock onto the biggest halo, because here the gas motion is governed by subsonic turbulence, see also Figure 7.
out in post-processing, the same procedure as used by Ryu et al. (2003) and Skillman et al. (2008). We can justify the simplicity of this approach by the marginal contribution made by shocks with low preshock temperature and density (voids onto filaments) to the dissipated energy, which is the main quantity of interest in our analysis. Nevertheless, reionization in post-processing could of course be modelled in a more sophisticated way, for example by a fitting function in the density-temperature plane (Vazza et al. 2009).

4.4 General Properties

In Figure 4 we present the state of the Illustris-NR-2 simulation at redshift $z = 0$. The projections were created by means of point sampling, and the shown quantities are the mass-weighted temperature, the mean baryonic overdensity, the Mach number weighted with the dissipated energy, and the mean dissipated energy density. The latter two are displayed only for the top left quarter of the former projections, which shows a supercluster including the biggest halo of the simulation. This halo has a mass of $M_{200,cr} = 3.2 \times 10^{14} \, M_\odot$, corresponding to a virial radius of $r_{200,cr} = 1.4 \, \text{Mpc}$.

Note that due to the temperature floor applied in post-processing only the hottest filaments are detected by the shock finder and are hence present in the bottom panels. We can clearly observe the well-known fact (Ryu et al. 2003) that high Mach numbers ($M \sim 10 - 100$) are generated at external shocks involving pristine preshock gas ($T_{\text{pre}} \lesssim 10^5 \, \text{K}$), whereas gas previously processed by internal shocks ($T_{\text{pre}} > 10^5 \, \text{K}$) experiences typically lower Mach numbers ($M \lesssim 10$). The density inside the supercluster exceeds the density of the voids by several orders of magnitude and thus the energy dissipation is most effective internally. The highest dissipation rate in this projection is present in the accretion shock onto the biggest cluster, whereas we do not detect many shocks inside the accretion shock.

4.5 Shock Statistics

Figure 5 quantifies the shock distribution and the associated energy dissipation in the Illustris-NR-2 run. In the left panel, the differential shock surface area normalized by the simulation volume is plotted as a function of the Mach number. We find redshift independently that 50% of the shocks have Mach numbers below $M = 3$, and 75% below $M = 6$. Towards lower redshift the cumulative area of shocks increases, especially for strong shocks. At redshift $z = 6$, shocks with a Mach number smaller than $M = 12$ account for 99% of all the shocks, whereas at $z = 0$ all the shocks up to $M = 35$ make up 99%. At low redshift, the accretion from previously unshocked gas onto hot filaments and cluster outskirts provides Mach numbers up to $M \approx 100$. At redshift $z = 0$, the total shock surface area reaches a value of $S = 2.5 \times 10^{37} \, \text{Mpc}^2$ (integral of the blue curve).

The right panel of Fig. 5 shows the differential thermal energy flux as a function of the Mach number. The total dissipated energy increases with time up to $z = 0.5$ and drops thereafter slightly to a value of $2.3 \times 10^{39} \, \text{erg} \, \text{s}^{-1} \, \text{Mpc}^{-3}$ (see also Fig. 3, but be aware of the factor $h^3$). The increase in time is expected due to an increasing number of shocks and the ever higher preshock densities and temperatures found inside structures. At low redshifts, this effect saturates and, furthermore, dark energy slows structure growth and dilutes the preshock gas inside voids, which leads to a drop of the thermal energy flux for high Mach numbers. The latter observation has also been pointed out by Skillman et al. (2008).

We find that 50% of the total energy dissipation occurs in shocks with $M < 4$, and 75% in shocks with $M < 6$. Mach numbers above $M > 40$ do not contribute significantly to the dissipation. We find that the energy dissipation peaks for $z = 0$ at $M \approx 2.3$ and shifts towards $M \approx 2.7$ for $z = 0$. This peak position at redshift zero differs considerably from the value $M \approx 2$ found by different previous studies (Ryu et al. 2003; Pfrommer et al. 2006; Skillman et al.

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Figure 6. Contribution of different baryonic preshock overdensities (top panels) and preshock temperatures (bottom panels) to the overall energy dissipation in the Illustris-NR-2 run. We find that most of the energy dissipation at \(z = 0\) is due to shocks with preshock overdensities in the range \(\delta_b \in (10^4, 10^5)\). Furthermore, around 70% of the total dissipation is contributed by preshock gas with temperatures \(T \in (10^7, 10^8)\), of which most is located in the WHIM.

| Temperature range [in K] | \(\delta_b < 10^1\) | \(10^1 \leq \delta_b < 10^2\) | \(10^2 \leq \delta_b < 10^3\) | \(\delta_b \geq 10^3\) |
|--------------------------|-----------------|-----------------|-----------------|-----------------|
| \(T \leq 10^4\) | 2% | 4% | 6% | 0% |
| \(T \in (10^4, 10^5)\) | 1% | 6% | 22% | 3% |
| \(T \in (10^5, 10^6)\) | 0% | 2% | 20% | 15% |
| \(T \geq 10^6\) | 0% | 1% | 7% | 10% |

Table 2. Contributions to the total energy dissipation for different preshock temperature and baryonic overdensity ranges at redshift \(z = 0\). We find that \(\approx 38\%\) of the energy gets dissipated by preshock gas of the WHIM (\(T \in (10^7, 10^8)\), \(\delta_b < 10^6\)), and \(\approx 57\%\) of the thermalization happens in clusters and groups (\(\delta_b \geq 10^5\)).

Previously unshocked cold gas accretes in strong external shocks but accounts only for a small amount of the dissipated energy. On the other hand, gas which gets shocked multiple times and is thus located inside structures produces low Mach number shocks with high energy dissipation. At zero redshift, gas with preshock temperatures \(10^5 \leq T < 10^7\) accounts for 69\% of the energy dissipation. Moreover, in order to determine the contribution of the warm-hot intergalactic medium, we examine the density of the gas in this preshock temperature range and find that \(\approx 54\%\) has a baryonic overdensity below \(\delta_b = 100\). A detailed break-up of the dissipation rates in different bins of preshock density and temperature is given in Table 2.

We interpret our findings as follows. Almost 40\% of the thermalization happens when gas from the WHIM gets shock heated, whereas shocks inside the accretion shocks of clusters and groups (\(\delta_b > 100\)) account for \(\approx 60\%\) of the dissipation. Thus, the relative importance of the WHIM is significantly higher than what has been found in previous studies. Furthermore, the shocks we identify in clusters and groups are prominent merger shocks rather than stemming from halo-filling, complex flow patterns, as shown in the next section.

4.6 Galaxy Cluster Shocks

Figure 7 shows zoom-projections of width 100 kpc around different massive halos of the Illustris-NR-2 simulation. The eight chosen halos are sorted by mass, and we show the baryonic overdensity as well as the energy dissipation by shocks. The white circle indicates the virial radius \(r_{200,\nu}\). The first halo is the biggest halo in the simulation and is also present in Fig. 4. As can be seen in the gas projection, there are turbulent motions inside the virial radius.

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However, we do not find many shocks inside this region, which points towards predominantly subsonic turbulence.

The third halo is in a state similar to the bullet cluster. The small subcluster ploughs through the gas of the big halo and produces a bow shock where a lot of energy is dissipated. The Mach number along the bow shock is $2 \lesssim M \lesssim 3.5$, comparable to the value $M = 3 \pm 0.4$ measured for the bullet cluster system (Markevitch et al. 2002; Markevitch 2006). The shocks in halos four and five form interesting spiral structures. These shocks might point towards the following scenario: A minor-merger event triggers gas sloshing and the formation of a spiral cold front (Ascenzi-bar & Markevitch 2006; Markevitch & Vikhlinin 2007; Roediger

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**Figure 7.** Zoom-projections with a width of 100 kpc centred on some of the biggest halos in the Illustris-NR-2 simulation. The top panels show the baryonic overdensity while the bottom panels indicate the energy dissipation. Accretion shocks onto the halos can be found close to but outside of $r_{200, cr}$ (white circles). Inside the accretion shocks prominent merger shocks are present. We do not find many shocks due to complex flow patterns within clusters, unlike reported by previous studies.
Figure 8. The radial shock surface distribution in several of the halos of Figure 7 (coloured lines, as labeled) as well as the average distribution of the 1000 largest halos in the Illustris-NR-2 simulation, stacked at redshift \( z = 0 \). The average dissipation profile has a peak at around \( R = 1.3 \) in units of the virial radius, which can be interpreted as the typical radius of the accretion shocks.

Figure 9. Top panel: Mach number dependent energy distribution for accelerating cosmic rays according to the DSA simulations of Kang et al. (2007). The black line shows the total kinetic energy processed by shocks per time and volume, while the red and blue curves give the fractions expected for particle acceleration with and without preexisting cosmic rays, respectively. Bottom panel: Contribution of different baryonic preshock overdensities to the total energy used for cosmic ray acceleration.

4.7 Cosmic Ray Acceleration

In this section, we discuss the role of the detected shocks in the Illustris-NR-2 run as cosmic ray (CR) sources. Collisionless cosmological shocks can inject cosmic rays through the diffusive shock acceleration mechanism (DSA; Blandford & Ostriker 1978; Malkov & O’C Drury 2001), also known as first order Fermi acceleration. In this process, ions with high thermal energies can diffuse upstream after crossing a shock and gain in a repetitive way in multiple shock crossings more and more energy. The cosmic ray injection efficiency depends strongly on the Mach number as well as on the level of Alfvén turbulence, and is most efficient if the magnetic field is parallel to the shock normal. Simulations of this DSA scenario were carried out by Kang et al. (2007), providing upper limits for the cosmic ray acceleration efficiency \( \eta(M) = f_{\alpha}/f_{\epsilon} \) of cosmological shocks, where \( f_\alpha \) is the processed kinetic energy flux, and \( f_\epsilon \) the energy flux transferred to cosmic rays.

The kinetic energy processed by shocks as well as the estimated available energies for cosmic ray acceleration at redshift \( z = 0 \) are presented in the top panel of Figure 9. The total inflowing kinetic energy amounts to \( 1.14 \times 10^{41} \mathrm{erg} \, \mathrm{s}^{-1} \, \mathrm{Mpc}^{-3} \). Without a preexisting cosmic ray population most of the acceleration energy is available in shocks with Mach numbers \( M \approx 3.2 \) (blue curve). Furthermore,
if we compare the integrals of the distributions, we estimate that ≈ 6% of the total kinetic energy processed by shocks is transferred into cosmic rays. In case of preexisting cosmic rays, which are generated in shocks at earlier times, the DSA mechanism is more efficient, especially for low Mach numbers (red curve). For this scenario, we find a peak position at $M \approx 2.5$ and a kinetic energy transfer to cosmic rays amounting to ≈ 18%.

In order to determine the spatial origin of the cosmic rays, we show the contributions of different baryonic overdensities to the total cosmic ray energy in the bottom panel of Fig. 9. For both scenarios (with and without preexisting cosmic rays) most of the energy transfer into cosmic rays is located in regions with densities $10 \leq \delta_b < 10^3$ ($\approx 68\%$). Without a preexisting population, only 43% of the cosmic ray energy is generated inside clusters and groups ($\delta_b > 100$). On the other hand, preexisting cosmic rays increase the efficiency for low Mach number shocks, which are mainly present inside dense structures. In this case we find that 58% of the energy for cosmic ray acceleration is provided by shocks inside clusters. We conclude that cosmological shocks could produce a significant amount of cosmic rays. Furthermore, the relevant shocks are shared in comparable proportions among both, regions with overdensities above and below $\delta_b = 100$.

5 METHODOLOGY VARIATIONS

In this section, we turn to an investigation of the origin of the discrepancies between our results and previous studies. For this purpose, we in particular investigate the shock zone determination criteria as well as the Mach number calculation approach for shock detection in the Illustris-NR-2 run.

For calculating the Mach number of shock surface cells, we normally evaluate pre- and postshock temperatures of cells just outside the shock zone. An exception to this are overlapping shock zones, in which case the preshock temperature is taken inside the combined shock zone and between the shock surfaces. Note that with this procedure, Mach numbers are calculated across a variable number of cells (variable jump range), depending on the extent of the imprint of the shock on the primitive variables. In the left panel of Figure 10, we show how the inflowing kinetic energy distribution as well as the dissipated energy distribution changes when we adopt a fixed jump range instead of calculating the Mach number always from the directly adjacent cells of a shock centre (short jump). Both distributions are shifted towards slightly lower Mach numbers. This finding is expected since a short jump does not fully enclose the broadened shock, and should hence lead to a smaller jump in the measured temperatures. For the dissipated energy distribution we find a peak shift from $M \approx 2.7$ to $M \approx 2.2$ as well as a reduction of the total dissipated energy by $\approx 15\%$ when the short jump is adopted.

In the next test we compare our default implementation of shock zone finding to a method in which the requirement for a minimum pressure jump ($\Delta \log p \geq \log p_{\text{th}}$) is abandoned, and the criterion $\nabla T \cdot \nabla p > 0$ is replaced with $\nabla T \cdot \nabla S > 0$. These relaxed criteria have been frequently used in previous studies and only recently Hong et al. (2014) suggested a replacement of the temperature-entropy criterion.

In Figure 11, we visualize the differences by applying the two methods to the Illustris-NR-2 simulation, omitting a temperature floor here for the purposes of this comparison test. With the old standard shock finding method (right panel), many more low Mach number shocks are found inside the WHIM and inside galaxy clusters. The additional shocks increase the total energy dissipation and...
Figure 11. Demonstration of the difference between our default shock finder implementation (left panel) and the old standard method (right panel). With the former implementation many more shocks are found inside the WHIM and inside clusters. These shocks are spurious as demonstrated in Figure 12. Depending on the applied evaluation method for the shock strength, some of the spurious shocks can be suppressed as shown in the right panel of Figure 10. Nevertheless, if spurious shocks enter the analysis the relative contribution of clusters to the total dissipated energy is overestimated. Note that for this comparison we do not adopt a temperature floor and thus find more shocks and higher Mach numbers compared to Figure 4.

We demonstrate in Figure 12 that the additional shocks are spurious by applying the old method to a three dimensional Kelvin-Helmholtz simulation in which no shocks are present. However, the old implementation is not able to filter tangential and contact discontinuities reliably in the shock zone determination, and thus false positive shocks are found along the density jump.

Depending on the applied scheme for assessing the shock strength (temperature jump, density jump or velocity jump), some of the spurious shock detections are suppressed by the consistency check that requires a correct jump direction in the shock surface determination (Section 2.3.3). The energy dissipation inferred for the different methods and different jump evaluations are presented in the right panel of Figure 10. Note that the reionization model through a temperature floor is disabled here, and we therefore obtain a tail towards very high Mach numbers. It can be seen that the old standard shock finding method is very sensitive to the adopted jump quantity for inferring the Mach number, while our new method is rather stable. There is good agreement between the temperature jump and velocity jump methods, whereas the pressure jump evaluation shifts the Mach numbers towards higher values for very strong shocks.

The old standard method in combination with the temperature jump gives clearly wrong results that are associated with an overestimate of the energy dissipation, which can be clearly seen from the difference of the dashed and the solid red line. By using the velocity jump instead, spurious shocks can be removed if the jump

Figure 12. Application of the previous standard shock finding method to a three dimensional Kelvin-Helmholtz instability simulation. This method does not filter tangential and contact discontinuities and thus finds spurious shocks even though this subsonic problem is formally free of shocks. Our new implementation on the other hand does not find shocked cells in the simulation volume, as desired.

the relative contribution of clusters due to high preshock densities and temperatures.
direction of the normal velocities is not consistent with the shock direction (temperature gradient). However, there remain then still a significant number of cases with wrong shocks detections, both with low and high Mach numbers (green dashed line). Note that the pressure jump across such spurious shocks is very small such that only a small Mach number is assigned if the pressure discontinuity is used to measure the shock strength. However, the distribution of energy dissipation at high Mach numbers is also altered compared to our default method, and perhaps surprisingly it is lower in this case (blue dashed line). The origin of this effect lies in the modification of the Mach number of real shocks by spurious shocks. This happens whenever the shock zone of a real shock gets modified (extended) by the shock zone of a spuriously detected shock nearby.

We conclude that the use of a variable jump range gives a small improvement compared to a fixed small jump range. It is yet more important to properly filter against tangential and contact discontinuities already in the shock zone determination to robustly avoid spurious shock detections and distortions in the resulting shock statistics.

6 SUMMARY

We have implemented a parallel shock finder for the unstructured moving-mesh code AREPO, based on ideas of previous work (Ryu et al. 2003; Skillman et al. 2008; Hong et al. 2014) combined with new refinements. Shocks are detected in a two step procedure. First, a broad shock zone is determined by analysing local quantities of the Voronoi cells to identify regions of compression. In a second step, a shock surface is identified by finding cells with the maximum compression across the shock zone, followed by an estimate of the Mach number through measuring the temperature jump across the shock zone. In this way, the Mach number is calculated over a variable number of cells which adjusts to the numerical broadening of the particular shock.

Improvements to previous methods have been realized by handling overlapping shock zones and by carefully filtering out tangential discontinuities and contacts in the shock zone determination. Such discontinuities are abundantly present in cosmological simulations, for example in the form of cold fronts and in shear. Such discontinuities are abundantly present in cosmological simulations, where we can identify all strong shocks reliably and account accurately and in a numerically converged way for the bulk of significant dissipation in shocks. At zero redshift, the energy dissipation measured with our shock finder for the adopted cosmological parameters is measured to be $2.3 \times 10^{60} \text{ erg s}^{-1} \text{ Mpc}^{-3}$.

Interestingly, we detected rich shock morphologies in the high resolution non-radiative simulation Illustris-NR-2. In particular, high Mach number accretion shocks onto filaments and cluster outskirts nicely trace the cosmic web. Accretion shocks onto galaxy clusters dissipate a lot of energy, while merger shocks inside the clusters give hints about their recent formation history. We note that the merger shocks appear as rather prominent and distinct features, whereas we do not find complex flow shock patterns inside the cluster accretion shocks, suggesting that there the gas dynamics is mostly characterized by subsonic turbulence (which we expect to be well captured by AREPO; Bauer & Springel 2012).

With our improved methodology, we find quantitatively revised results for the shock dissipation statistics in non-radiative cosmological simulations. Most of the thermalization happens in shocks with Mach numbers around $M \approx 2.7$. Moreover, almost 40% is contributed by shocks in the WHIM and $\approx 60\%$ by shocks in clusters and groups. Compared to previous studies, these findings correspond to a shift in the energy dissipation spectrum towards higher Mach numbers and towards structures with lower densities. Also, we have found $R = 1.3 \times r_{200,c,\text{vir}}$ as a typical radius for accretion shocks onto galaxy clusters at redshift $z = 0$, based on identifying a peak when stacking the radial shock dissipation profiles of 1000 halos of the Illustris-NR-2 simulation. Consequently, the accretion shock is expected to typically lie slightly outside the virial radius, a finding which is consistent with Battaglia et al. (2012). We note however that the accretion shock position shows a high degree of temporal variability in any given halo.

Finally, we also investigated the expected energy transfer to cosmic rays in the identified large-scale structure shocks if acceleration efficiencies derived from diffusive shock acceleration plasma simulations are adopted (Kang et al. 2007). These simulations are set up with a magnetic field parallel to the shock normal direction and provide therefore upper limits for the acceleration efficiency. We obtain at redshift $z = 0$ an average cosmic ray energy injection rate of $7.0 \times 10^{49} \text{ erg s}^{-1} \text{ Mpc}^{-3}$ in the case of non-preexisting cosmic ray populations, and a considerably larger value in the case of pre-existing cosmic rays. Considering these numbers, it is quite plausible that even for random magnetic field orientations a dynamically important cosmic ray population is produced in these shocks. Furthermore, we found that gas with preshock overdensities above and below $\delta_0 = 100$ contribute roughly equally to the energy transfer into cosmic rays.

In future work, it will be interesting to couple the shock finder to hydrodynamical simulations that take cosmic rays self-consistently into account. Also, it should be interesting to contrast the results obtained here for non-radiative simulations with an analysis of full physics simulations of galaxy formation that include radiative cooling and heating mechanisms, as well as prescriptions for star formation, stellar evolution, black hole growth and associated feedback processes. These simulations feature interesting additional shocks, for example due to strong feedback-driven outflows. In a companion paper (in preparation), we will present an analysis of the corresponding shocks in the recent Illustris simulation (Vogelsberger et al. 2014a).
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