NONEQUILIBRIUM THERMODYNAMICS AND COSMOLOGICAL PANCAKE FORMATION

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ABSTRACT

We investigate the influence of nonequilibrium thermodynamics on cosmological structure formation. In this paper, we consider the collapse of the planar perturbations usually called “Zeldovich pancakes.”

We have developed for that purpose a new two-fluid (gas and dark matter) hydrodynamical code, with three different thermodynamical species: electrons, ions, and neutral particles, $T_e \neq T_i \neq T_n$. We describe in detail the complex structure of accretion shock waves. We include several relevant processes for a low-density, high-temperature collisional plasma: nonequilibrium chemical reactions, cooling, shock heating, thermal energy equipartition between electrons, ions, and neutral particles, and electronic conduction. We find two different regions in the pancake structure: a thermal precursor ahead of the compression front and an equipartition wave after the compression front, where electron and ion temperatures differ significantly. This complex structure may have two interesting consequences: preheating of unshocked regions in the vicinity of massive X-ray clusters and ion and electron temperature differences in the outer regions of X-ray clusters.

Subject heading: cosmology: theory — hydrodynamics — methods: numerical

1. INTRODUCTION

The thermodynamical state of the intergalactic medium is of primary importance in the study of the formation and evolution of cosmic structures. In the dense central regions of galaxy clusters, cooling is likely to play a dominant role. In the outer regions, the density is rather low and allows an adiabatic treatment of gas dynamics. At the same time, non-equilibrium thermodynamics occurs in this hot and diffuse adiabatic treatment of gas dynamics. At the same time, non-equilibrium thermodynamics occurs in this hot and diffuse plasma. Indeed, for high temperatures ($T \approx 10^8$ K) and low densities ($n_e \approx 10^{-4}$ cm$^{-3}$), typical values found in the outer regions of large X-ray clusters (Markovitch et al. 1996), the timescale for electrons and ions to reach thermodynamical equilibrium through Coulomb collisions is about $t_{ei} \approx 4 \times 10^9$ yr, comparable to the Hubble time.

It has been pointed out by Kang et al. (1994) that an Eulerian code is well suited to studying these low-density regions, where a strong departure from thermodynamical equilibrium is expected. In this paper, we therefore present a new Eulerian code, and then use it to model nonequilibrium processes during the formation of Zeldovich pancakes.

Pancakes have appeared for a long time as fundamental tools in cosmology. Zeldovich (1970) was the first to point out that sheetlike structures could form through gravitational instability. These pancakes were first motivated by the neutrino-dominated scenario of structure formation, in which they form naturally. Although this scenario seems today to be in difficulties with current observations, walls and filaments are still observed in both observational and theoretical studies based on other, more popular scenarios, such as cold or mixed dark matter (Cen & Ostriker 1992; Peebles 1993). Therefore, pancake geometry is not just an idealized case for testing numerical codes, but is also cosmologically relevant.

The hydrodynamics of pancake collapse have been studied by several authors (Bond et al. 1984; Shapiro & Struck-Marcell 1985; Anninos & Norman 1994), with the baryon component obeying the hydrodynamic equations and coupled to collisionless dark matter particles. Different numerical schemes for modeling the hydrodynamical equations have been used. Bond et al. (1984) and Anninos & Norman (1994) used an Eulerian scheme, while Shapiro & Struck-Marcell (1985) used a Lagrangian scheme. All these studies were dedicated to the calculation of the cooled mass fraction formed via pancake collapse. Contrary to previous studies, we focus in this paper on nonequilibrium phenomena that are enhanced in the large-scale, low-density parts of pancakes. We introduce three temperatures to describe the thermodynamic evolution of electrons, ions, and neutral particles. Chemical evolution of the primordial hydrogen-helium gas is solved without assuming ionization-recombination equilibrium. We also model electronic conduction with a flux-limited diffusion scheme.

This paper is organized as follows. In § 2 we present the basic equations governing the system and describe our hydrodynamical code, with validating tests. In § 3 we present the results of simulations concerning the formation of pancakes. We show that in the general case, a complex structure forms, with a thermal wave escaping out of the shocked region together with an equipartition wave, where electron and ion temperatures can differ significantly. Finally, in § 4 we discuss the roles of various parameters, such as the baryon density parameter $\Omega_B$, the wavelength of the initial perturbation $\Lambda$, and the pancake collapse epoch $a_c$.

2. PHYSICS AND NUMERICAL METHODS

2.1. Basic Equations

The equations are written in comoving coordinates, through the transformation $r = a(t)x$, where $a(t)$ is the expansion factor. We here take $a$ as the time variable. We assume an Einstein–de Sitter universe, with zero cosmological constant. The velocities of dark matter particles and...
fluid elements are, respectively, $v = dx/da$ and $u = dx/da$. Dark matter particles satisfy the equations of motion,
\[
\frac{dv}{da} = -\frac{2 - \Omega/2}{a} - \frac{3\Omega}{2a^2} v - \frac{3\Omega}{2a^2} V_x \phi ,
\]
where $\Omega$ is the background density parameter and $H$ is the Hubble constant (both parameters are time-dependent quantities). For Lagrangian fluid elements, one has to add the pressure term
\[
\frac{du}{da} = -\frac{2 - \Omega/2}{a} u - \frac{3\Omega}{2a^2} V_x \phi - \frac{1}{a^2 H^2} \rho_b
\]
and consider the continuity equation
\[
\frac{1}{\rho} \frac{d\rho}{da} = -\left(\frac{3}{a} + V_x \cdot u\right).
\]
The total pressure, $P = P_e + P_i + P_n$, is the sum of the electron, ion, and neutral particle partial pressures. The gravitational potential satisfies the Poisson equation
\[
V_x^2 \phi = \frac{\rho - \bar{\rho}}{\rho} = \delta ,
\]
where $\rho = \rho_e + \rho_i + \rho_n$ is the total mass density and $\bar{\rho}$ is the mean background total mass density. Throughout this paper, densities refer to proper physical quantities and not to comoving quantities. We consider six chemical species, with number densities of each species $n_e$, $n_{\text{He}^+}$, $n_{\text{H}^+}$, $n_{\text{He}}$, $n_{\text{He}^+}$, and $n_{\text{He}^+}$. The partial pressures are then related to the kinetic temperatures as $P_e = n_e k T_e$, $P_i = (n_{\text{He}^+} + n_{\text{He}} + n_{\text{He}^+}) k T_i$, and $P_n = (n_{\text{He}^+} + n_{\text{He}}) k T_n$. We define the specific volume $V = 1/\rho$, occupied by a unit mass of baryons. The specific internal energy $E_x$ for each thermodynamical species ($x = e, i, n$) then follows the equation of state for a monoatomic gas ($\gamma = 5/3$),
\[
E_x = \frac{1}{\gamma - 1} P_x V ,
\]
and satisfies the first law of thermodynamics,
\[
\frac{dE_x}{da} = -(\gamma - 1)E_x \left(\frac{3}{a} + V_x \cdot u\right) + \frac{d\rho}{da} .
\]
The first term in the right-hand side of equation (6) is the $PdV$ work from expansion and comoving compression, and the last term is the net heat source per unit mass from different irreversible, nonadiabatic processes.

2.2. Thermodynamical Processes

The thermodynamical evolution of the plasma is treated in a self-consistent way with its chemical evolution, without assuming ionization-recombination equilibrium. The thermodynamical processes modeled in our code are shock heating for ions and neutral particles, cooling and thermal conduction for electrons, and equipartition between electrons, ions, and neutral particles.

We have used the collisional ionization rate and the radiative recombination rate given by Cen (1992), which include correction terms for very high temperatures. As we have to deal with three different kinetic temperatures for the gas, the actual rates are obtained by using the reduced temperature of the two reactants (Draine 1980; Draine & Katz 1986). In the case of proton-electron interaction, this gives us $T_{ei} = (n_e T_e + n_i T_i)/(n_e + n_i)$. In practice, if $T_e \approx T_i$, this implies a small correction of the order of $n_i/n_e$. But in some extreme cases, where $T_i \gg T_e$, this correction is not negligible. We also considered classical cooling processes such as ionization, recombination, and line cooling, together with bremsstrahlung and Compton cooling by the cosmic background radiation. The cooling rates are again those of Cen (1992), modified using the reduced temperature. Note that cooling results in an internal energy loss for the electrons only.

Massive particles (ions and neutral) share most of the entropy deposition from shock heating. The electrons are mainly heated by energy exchange with the latter species. As a matter of fact, in a perfect fluid, shocks are discontinuities in the flow, obeying Rankine-Hugoniot relations. This implies that the postshock temperature for a given particle species $i$ is $T \approx m_i D^2$, where $D$ is the upwind fluid velocity in the rest frame of the shock front. Consequently, the postshock electron temperature is $m_e/m_p$, much lower than the ion postshock temperature and negligible compared to the final equilibrium temperature. We therefore neglect electron shock heating. Shock heating will be treated in the code using the artificial viscosity method (Von Neuman & Richtmyer 1974), which includes a linear and a quadratic viscous term. This can be written in one dimension, and in one dimension only, as a viscous pressure, added to the usual ion (or, respectively, neutral particle) thermal pressure:
\[
P_{i,\text{visc}} = P_i (1 + 2\epsilon^2) ,
\]
where
\[
\epsilon = -\frac{\Delta x}{c_{ei}} (3 + a V_x \cdot u) .
\]
The equivalent energy-source term entering equation (6) for ions is given by
\[
\frac{d\rho_{i,\text{visc}}}{da} = -P_{i,\text{visc}} \left(\frac{3}{a} + V_x \cdot u\right).
\]
Similar equations apply for neutral particles. $C_1$ and $C_2$ are two constants determined a posteriori by numerical tests, and $\Delta x$ is the mesh spacing.

Electrons are heated by ions through Coulomb interactions, and by neutral particles through short-range forces. The equipartition rates are computed using the momentum transfer cross section of the different interacting species. For example, the net kinetic energy transfer rate per unit mass between electrons and protons is (Spitzer 1962)
\[
\frac{d\rho_{e-p}}{da} = -\frac{d\rho_{e-p}}{da} = -k (T_i - T_e)
\]
\[
\times \left[\frac{4(2\pi)^{1/2} e^4 m_e^{3/2} \ln \Lambda_{ep}}{m_p (k T_{ei})^{3/2}}\right] n_e n_p \rho_B aH ,
\]
where $T_{ei}$ and $\ln \Lambda_{ep}$ are the reduced temperature and the Coulomb logarithm of the two interacting particles, respectively. The heat transfer rates between the other chemical species can be expressed in a similar form (Draine 1980; Chièze, Pineau des Forêts, & Flower 1998b).

When electronic temperature gradients are present in the flow, a net heat flux appears, written here in its classical...
form,
\[ q_{\text{el}} = -\frac{1}{a} \kappa_e V_x T_e, \]  
(10)
with conductivity coefficient (Spitzer 1962)
\[ \kappa_e = 1.84 \times 10^{-5} \frac{T_e^{5/2}}{\ln \Lambda}. \]  
(11)

In the case of very high fluxes (very steep gradients or very high temperatures and low densities), the flux saturates to a value corresponding to a free transport of the electron internal energy at a fraction of the electron sound speed. We choose the flux-limited diffusion scheme described in Cowie & McKee (1977). The formulae we use here are
\[ q_e = \frac{q_{\text{el}}}{1 + q_{\text{el}}/q_{\text{sat}}}, \]  
(12)
where the maximum (saturated) value of the heat flux is given by
\[ q_{\text{sat}} = 0.4 \left( \frac{2kT_e}{m_e} \right)^{1/2} n_e kT_e. \]  
(13)

The heat source (or sink) that enters equation (6) because of electronic conduction is finally given by
\[ \frac{d \beta_e}{da} = -\frac{1}{a^2 \gamma} V_x \cdot q_e. \]  
(14)

Ions are also able to transfer heat through ion conduction, but the conduction coefficient is reduced by the factor \((m_i/m_e)^{1/2}\), so this extra heat flux is much less effective. Moreover, the average kinetic velocity for the ion gas after the shock front is lower than the shock velocity. Consequently, ions do not cross the shock front, except for a few suprathermal particles. The thermal flux due to ions is therefore neglected. On the other hand, the electron sound speed is \((m_e/m_i)^{1/2}\) times larger than the shock-wave velocity (Zel’dovich & Raizer 1966). The electron heat flux therefore easily crosses the compression front and efficiently preheats the cold gas ahead of the shock. Finally, ions will in turn be heated through Coulomb energy exchange with electrons.

The capacity of electrons to transport heat via conduction, but the conduction coefficient is reduced by the factor \((m_i/m_e)^{1/2}\), so this extra heat flux is much less effective. Moreover, the average kinetic velocity for the ion gas after the shock front is lower than the shock velocity. Consequently, ions do not cross the shock front, except for a few suprathermal particles. The thermal flux due to ions is therefore neglected. On the other hand, the electron sound speed is \((m_e/m_i)^{1/2}\) times larger than the shock-wave velocity (Zel’dovich & Raizer 1966). The electron heat flux therefore easily crosses the compression front and efficiently preheats the cold gas ahead of the shock. Finally, ions will in turn be heated through Coulomb energy exchange with electrons.

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### 2.3. Numerical Techniques

We present here our one-dimensional hydrodynamical Eulerian code. The extension of this code to a fully three-dimensional hydrodynamical scheme is presented in a companion paper (Chièze, Alimi, & Teissier 1998a).

Our code is based on the operator-splitting method, with four consecutive steps. The first step is called the gravity step. This solves the Vlasov-Poisson equations for dark matter particles and calculates the gravitational potential. The second step is called the Lagrangian step; this solves the adiabatic hydrodynamic equations in their Lagrangian form. The third step is called the Eulerian step; here we calculate the projected hydrodynamic quantities on the fixed Eulerian grid from the perturbed Lagrangian grid. The last step is called the dissipative step; in this step we compute all the local dissipative processes cell by cell, using the densities derived in the two previous steps. Our code in its final version is of second-order accuracy in both time and space. It allows great stability and efficiency. We present here its general features. We then show tests that demonstrate its ability to handle cosmological simulations.

### 2.4. General Presentation of the Code

We consider a two-fluid system (dark matter and baryons). The physical variables associated with dark matter particles (superscript \(\star\)) are \(x^i\), the position of particle \(j\), and \(v^j\), the velocity of particle \(j\). The discrete values of the flow on the grid (superscript \(\bar{\cdot}\)) are \(M^i\), the total baryon mass in cell \(i\); \(N_X^i\), the total numbers of particle \(X\) in cell \(i\); \(S_e^i, S_i^i, S_\mu^i\), respectively the total entropy of electrons, ions, and neutral particles in cell \(i\); \(u_x^i, u_y^i\), the velocity in the x-direction of interface \(i\); and finally \(r_x^i\), the position in the x-direction of interface \(i\).

Mass, particle numbers, and entropies are zone-centered, while the velocity is face-centered. This is the well-known staggered-mesh method (Stone & Norman 1992). It allows better accuracy when computing finite differences, and also reduces the number of interpolations needed to calculate fluxes, which are defined at cell interfaces. The variable \(r_x^i\) is usual in pure Lagrangian schemes; it allows us to compute densities while the mass remains constant. As we will see below, it also improves the accuracy of both time integration and flux interpolation.

The specific entropy, \(S_{\text{e}}\), is defined for each thermodynamical species \(x\) as \(S_x = E_x / V_x^{\gamma - 1}\). Using the energy equation (6), the time derivative of \(S_x\) reduces to
\[ \frac{dS_x}{da} = \frac{S_x d \beta_x}{E_x da}. \]  
(15)

The thermodynamical evolution of baryons is computed using the entropy equation (15) rather than the energy equation (6). This method does not introduce any numerical spurious dissipation effects of expansion or compression. Consequently, an adiabatic flow \((d \beta_x / da = 0)\) is strictly adiabatic during the Lagrangian step.

### 2.5. Gravity Step

We evolve the dark matter particles using a particle-mesh algorithm (Hockney & Eastwood 1981) with a predictor-corrector scheme. This time integrator ensures both second-order time accuracy and variable time stepping. Let us suppose that particle positions and velocities are known at a given time \(a\). We compute the predicted positions at time \(a + \Delta a\) with \((x^j)^{\star 1} = x^j + \Delta av^j\). The superscript \(\star\) means that the quantity is the predicted quantity evaluated at time \(a + \Delta a\). The dark matter density fields \(\rho^i\) and \(\left(\rho^i\right)^{\star 1}\) are then evaluated with a CIC interpolation scheme. In order to solve the Poisson equation, we also need to know the predicted baryon density field, \(\left(\rho_b^i\right)^{\star 1}\). This is deduced from the baryon density and velocity fields at time \(a\) by solving the continuity equation. From the gravitational potential \(\phi\) at time \(a\) and from its predicted quantity \((\phi)^{\star 1}\) at time \(a + \Delta a\), we deduce the forces \(F^j\) and \((F^j)^{\star 1}\) for the dark matter par-
icles by inverse interpolation at respectively positions \( x'^i \) and \( (x')^{(2)} \). Velocities and positions for dark matter particles are finally updated according to the formula

\[
\frac{(v')^{(2)} - v'}{\Delta a} = -2 - \frac{\Omega/2}{\Omega} (v')^{(2)} + v' - \frac{3\Omega}{2a^2} F + (F')^{(1)},
\]

(16)

\[
\frac{(x')^{(2)} - x'}{\Delta a} = (v')^{(2)} + v',
\]

(17)

where \( a \) is now the centered expansion factor \( a + \Delta a/2 \), \( \Omega \) is the corresponding density parameter, and \( (x')^{(2)} \) and \( (v')^{(2)} \) are the updated position and velocity for particle \( j \) at time \( a + \Delta a \).

### 2.6. Lagrangian Step

At this step we solve the adiabatic hydrodynamics equations, together with shock heating and electronic conduction. All the quantities involved in these equations depend on spatial derivatives of the flow. These are estimated with a finite-difference scheme. Chemical cooling and equipartition processes that are purely local (i.e., that do not depend on spatial derivatives of the flow) are solved in the dissipative step.

We write the adiabatic hydrodynamic equations for interface \( i \) for an explicit scheme [first-order, designated by superscript (1)] as

\[
\left( \frac{\Delta x}{\Delta a} \right)_i^{(1)} = u'_x,
\]

(18)

\[
\left( \frac{\Delta u_x}{\Delta a} \right)_i^{(1)} = -2 - \frac{\Omega}{2} u'_x - \frac{\Omega}{2a^2} \frac{\phi' - \phi'^{-1}}{\Delta x} - \frac{2\Delta x^2}{aH^2} \frac{P'_i - P'^{-1}}{M'_i + M'^{-1}},
\]

(19)

where the pressure \( P'_i \) includes electron, ion, and neutral partial pressures and the artificial viscous pressures for shock heating (eq. [7]). The entropy equations for electronic conduction for electrons and for shock heating for ions and neutral particles for the cell \( i \) are derived in a similar way from finite differencing of equations (8), (12), and (15). Only the variables \( (r'_x, u'_x, S'_i, S'_n, S'_{ve}, i = 1, N) \) are coupled; the total mass and total numbers of particles remain strictly constant during the Lagrangian step. In order to integrate the previous equations, we need to compute the increments (designed by \( \Delta \)) of each variable between time \( a \) and time \( a + \Delta a \). Several methods are possible. The most straightforward is to use directly the explicit estimation we already mentioned (the first-order method; see Stone & Norman 1992). However, this needs a rather strong condition on the time step in order to be stable; namely, the Courant condition. The implicit method, on the other hand, allows much larger time steps. It is very stable, but very CPU time consuming, because it implies inverting a band matrix. In this paper, we prefer to use a second-order time integrator scheme inspired by the implicit method. This consists of deriving second-order increments by Taylor expanding the first-order increments given by equations (18) and (19) with respect to the flow variables, namely, \( r_x, u_x, S_i, S_n, \) and \( S_{ve} \). For example, the acceleration terms for interface \( i \), which depend on \( u'_{x-1}, r'_{x-1}, S'_{x-1}, S'_{n-1}, S'_{ve}, u'_x, r'_x, S'_i, S'_n, S'_{ve}, u'_x, r'_{x+1}, S'_{x+1}, S'_{n+1}, S'_{ve}, u'_{x+1} \), and \( r'_{x+1} \), yield the following second-order [superscript (2)] estimation of the velocity increment:

\[
\left( \frac{\Delta u_x}{\Delta a} \right)_i^{(2)} = \frac{1}{2} \left( \frac{\Delta u_x}{\Delta a} \right)_i^{(1)} + \Delta a \frac{\partial}{\partial \phi_x} \left( \frac{\Delta u_x}{\Delta a} \right)_i^{(1)} \left( 1 - \frac{\Delta a}{\Delta x} \right),
\]

(20)

where only the partial derivative with respect to \( r'_{x-1} \) and \( u'_{x-1} \) has been written for the sake of simplicity. It is important to add partial derivatives of the first-order increment with respect to all variables involved in equation (19). This method differs from the standard predictor-corrector scheme, since the second-order correction presented here is computed analytically using partial derivatives of the first-order increments. At the end of the Lagrangian step, we have the new entropies, the new velocities, and the new interface positions. Masses and numbers of particles have not been modified.

Finally, the time step is controlled using the usual methods (see, e.g., Stone & Norman 1992), with constraints for the artificial viscosity, conduction, gravity, and gas dynamics. For example, for a pure gas dynamics problem, the time step is controlled by

\[
\Delta a = C_0 \min \left( \frac{a^2 H \Delta x}{\sqrt{(a^2 Hu)^2 + c_s^2 + c_{visc}^2}} \right),
\]

(21)

where \( c_s \) is the adiabatic sound speed, and \( c_{visc} \) is related to the viscous pressure by the formula

\[
c_{visc} = 4 \sqrt{\frac{\gamma P_{visc}}{\rho_B}}.
\]

(22)

The factor 4 in the last equation corresponds to the stability criterion for a viscous fluid with constant viscosity coefficient \( \gamma \); the equations of motion in this case are analogous to the well-documented diffusion equation, for which the stability criterion is established as \( \Delta t \leq (\Delta x)^2/(4\gamma) \) (see Stone & Norman 1992). The Courant safety coefficient \( C_0 \) must be chosen to be less than 0.5 in order for an explicit (first-order) scheme to be stable, and even smaller (typically 0.1) for it to be accurate. In contrast, our second-order scheme remains stable and accurate even with the ultimately large time stepping given by \( C_0 = 1 \) (see § 2.9).

### 2.7. Eulerian Step

We now want to remap all variables from the disturbed Lagrangian grid to the fixed Eulerian one. This step must conserve mass, number of particles, internal energies of electrons, ions, and neutral particles, and momentum. We defined the left-centered momentum in cell \( i \) as \( P'_L = M'_i u'_i \) and the right-centered momentum in cell \( i \) as \( P'_R = M'_i u'_{i+1} \), in order to deal only with zone-centered quantities. The projection step then consists of solving the advection equation (written here only for the mass)

\[
\frac{\partial}{\partial t} \int \rho \, dV = - \int \rho \, u \cdot dS
\]

(23)
for each zone that has a control volume \( V^i = (\Delta x)^2 (r_{x+1}^i - r_x^i) \). A finite-difference approximation of this integral equation is

\[
M_p^i - M^i = \Delta M_x^i - \Delta M_x^{i+1},
\]

where \( M_p^i \) are the projected masses on the Eulerian grid and \( \Delta M_x^i \) is the advected mass through interface \( i \). This scheme is strictly conservative for the projected variables by construction. The main problem of the advection procedure arises when one calculates the total mass contained in the advected volumes. To do so, we must calculate a realistic mass distribution within each cell, and then integrate this distribution in the advected volume. There are basically three tractable methods: uniform, linear, and parabolic distributions. These three methods are known as the donor cell method, the Van Leer method (Van Leer 1977), and the piecewise parabolic interpolation (PPI) method (Woodward & Colella 1985). The first of these is very simple but quite diffusive. It is first-order accurate in space. The other two methods are much less diffusive and are respectively second- and third-order accurate in space. The PPI method is the most time consuming, while Van Leer method offers a good compromise between accuracy and efficiency (see Stone & Norman 1992 for a general description).

We calculate interpolation functions for mass, momentum, and total internal energy \((E = E_c + E_t + E_i)\) only. The number of particles within the cell are distributed according to the mass distribution, and internal energies for the three species are distributed according to the total internal energy distribution. This ensures exact mass and charge conservation within each cell, and avoids spurious decoupling between the three temperatures. The entropy values are then updated from the projected internal energy, and the velocity is updated from the left-centered projected momentum, the right-centered projected momentum, and the projected mass according to the formula

\[
u_i = \frac{P_{k,i}^{-1} + P_{L,i}}{M^{-1} + M_i}.
\]

This equation yields an exact momentum conservation. All new hydrodynamics variables on the Eulerian grid are now known.

2.8. Dissipative Step

We now solve cell by cell all purely local dissipative processes: chemical reactions, thermochemical energy exchanges, equipartition, and cooling. All these processes are described by very stiff equations. They imply necessarily very short time steps, which would dramatically slow down the whole simulation and increase the CPU time to prohibiting values. Consequently, to avoid this time step catastrophe, we solve these stiff equations by using \( n \) consecutive substeps. At each substep and for each cell, we invert a \( 6 \times 6 \) matrix for the chemical reactions of the six involved species and a \( 3 \times 3 \) matrix for the entropies. Our algorithm is fully vectorized and very effective, allowing high accuracy and stability. The number of substeps depends on the physical state of the cell. A similar method was used by Anninos & Norman (1994). However, this method is not justified as soon as the timescale of dissipative processes is much shorter than the dynamical timescale given by the Lagrangian step. This happens in very dense regions, where cooling can be overestimated. We discuss how to avoid such a mistake in Chieze et al. (1998a). In the Eulerian low-resolution case presented here, this happens in only one or two cells at the pancake center. However, using the prescription presented in Chieze et al. (1998a) (which consists essentially of turning off line cooling in the central cell only), we find that cooling at small scales has little influence on the large-scale flow.

2.9. Numerical Tests

2.9.1. Advection Test

This test was proposed by Stone & Norman (1992) to qualify the advection scheme only. We consider a box of length unity filled with a gas of homogeneous density. With a resolution of \( N = 512 \) cells and periodic boundary conditions, we model the advection at a constant velocity of a single square pulse of density \( 10 \), initially sampled by \( 50 \) cells. The results we obtain with the three different projection schemes are very close to those obtained by Stone & Norman (1992) at the time when the pulse has crossed half of the computational space. The donor cell interpolation is dramatically diffusive, while the other two schemes reproduce the sharp features relatively well.

2.9.2. Shock-Tube Test

This test, also called the classical Riemann problem, may be the most widely used test for qualifying hydrodynamics codes (Sod 1978). The initial conditions we use here are similar to those used by Stone & Norman (1992). We consider a box of size \( L = 1 \), \( N = 128 \) cells, and \( \mu = 0 \). We separate the box into two regions (left and right), with the following conditions: \( \rho_L = 1 \), \( p_L = 1 \), \( \rho_R = 0.125 \), \( p_R = 0.1 \). We assume \( \gamma = 1.4 \) and reflective boundary conditions.

For this test we use the quadratic term of the artificial viscosity only, with \( C_1 = 0 \) and \( C_2 = 3 \). In Figure 1, we plot the different profiles obtained at time \( t = 0.245 \) for our standard simulation parameters, namely a Courant safety factor \( C_0 = 0.5 \), the Van Leer advection scheme, and our second-order time integrator. The results of our code are comparable to other methods, and very close to the analytical solution. Note, however, that the specific energy in the post-shock region is slightly better reproduced here than for the example in Stone & Norman (1992). We think that this better agreement is mainly due to our second-order time integrator.

To analyze the effect of our second-order time integrator, we run the same simulation, but with a Courant safety factor \( C_0 = 1 \), which is the ultimate possibility. In Figure 2 we plot the specific energy profiles obtained at time \( t = 0.245 \) for the three different advection schemes (donor cell, Van Leer, and PPI) using the second-order time integrator, together with the profile obtained with the Van Leer advection scheme using the first-order explicit method.

Note that in this latter case the solution is strongly unstable, while for the three former cases, the solution is identical to the \( C_0 = 0.5 \) case. This illustrates the interest of our second-order time integrator. We also learn from this figure that the donor cell advection scheme is dramatically diffusive, and is of practically no use. The improvement of the solution between the Van Leer and PPI schemes is real but not very dramatic, although for the latter the computational cost is much higher. This justifies the use of the Van Leer method as a standard choice.
2.9.3. **Blast Wave Test**

This test was used by Woodward & Colella (1985) to compare different hydrodynamic codes. It may be the most frequently adapted test for cosmological applications, because strong shocks are generated with Mach numbers \( \simeq 10^3 \) and are interacting violently. The initial conditions we use are (see Stone & Norman 1992) \( L = 1, N = 1200 \) cells, \( \rho = 1 \), and \( u = 0 \). In the left tenth of the box, we put \( p = 1000 \), in the right tenth \( p = 100 \), and in the middle \( p = 0.01 \). We assume \( \gamma = 1.4 \) and reflective boundary conditions. For a more precise description of the different features involved in this simulation, see Woodward & Colella (1985). For this test, the linear term of the artificial viscosity is necessary to damp small oscillations otherwise occurring after strong shock fronts (we assume \( C_1 = 1 \) and \( C_3 = 3 \)). We consider a Courant safety factor \( C_0 = 0.5 \) and our second-order time integration scheme. Had we decided to use the first-order time integrator (explicit method), the Courant safety factor would have to be \( C_0 \approx 0.1 \) in order to recover similar results. We show in Figure 3 the density profiles obtained at time \( t = 0.038 \) to compare with those of Stone & Norman (1992) and Woodward & Colella (1985). At that time, the two shock waves have already interacted at \( x \approx 0.7 \) and are moving back to their original positions.

The PPI scheme presents the best agreement with the Woodward & Colella (1985) reference simulation, although Van Leer results appear to be very similar as well. As already mentioned, the donor cell scheme is unable to correctly handle sharp discontinuities, but more dramatic is the bad positioning of the shock fronts. During this run, the total energy conservation for donor cell, Van Leer, and PPI schemes was 7.6%, 2.1%, and 1.1%, respectively.

3. **PANCAKE COLLAPSE**

3.1. **Initial Conditions**

For all runs we take the same initial conditions, beginning at epoch \( z_i = 200 \), where matter and radiation are well decoupled. The total density contrast has the distribution

\[
\delta(x) = \frac{a_i}{a_e} \cos \left( \frac{2\pi x}{L} \right),
\]

and the baryon density distribution is taken to be \( \rho_B(x) = \rho_B[1 + \delta(x)] \). Dark matter particles then move according to the Zeldovich approximation, with the displacement field corresponding to the above density contrast. The initial velocity field for baryons is given by the linear growing mode,
Fig. 2.—Specific energy profiles obtained with the shock-tube test for different advection schemes, second-order time integration, and the “ultimate” Courant safety factor $C_0 = 1$. We also plot the solution obtained with the explicit method (first-order) for the same Courant safety factor. The analytic profile is shown as the solid line in each graph.

$$u_x(x) = -\frac{\Omega^{0.6}}{a} \partial_x \phi.$$  \hspace{1cm} (27)

The temperature for ions, electrons, and neutral particles is chosen to be uniform and equal to $T_{e,i,n}(x) = T_0(1 + z_i)$, where $T_0 = 2.7$ K is the cosmic radiation background temperature today. We suppose that the helium mass fraction is $Y = 0.24$. The initial ionization fractions are taken from Peebles (1993). In all our runs, we take $\Omega = 1$ and $H_0 = 50 \text{ km s}^{-1} \text{ Mpc}^{-1}$. Therefore, the single cosmological parameter of interest here is $\Omega_B$. We have adopted periodic boundary conditions to ensure total mass conservation. We used the Van Leer projection scheme, since it presents a good compromise between accuracy and CPU time cost, and we adopt a Courant safety factor $C_0 = 0.5$. We consider in the following discussion a reference pancake defined by a comoving length $L = 16 \text{ Mpc} h^{-1}$, a collapse epoch $a_c = 0.2$, and a baryon density parameter $\Omega_B = 0.1$.

3.2. Adiabatic Collapse

In this standard case, the gas is assumed to be fully ionized and described by a single kinetic temperature.
Sunyaev & Zeldovich (1972) and Bond et al. (1984) have analytically derived density and temperature profiles for such a case. They have shown that a shock wave appears off center at a very small radius (typically a few \(10^{-6}\) Mpc) corresponding to the sonic radius. The flow is almost hydrostatic in this inner, unshocked region of high-density contrast. The accretion shock front propagates outward, leaving an almost uniform pressure all over the accreted gas. Here, in contrast to Bond et al. (1984) and Shapiro & Struck-Marcell (1985), we do not resolve this very central region, because we are using a regular mesh (this mesh has been chosen so as to better describe the large-scale, outer region of the pancake). We are aware of the fact that the better the resolution, the higher the density contrast will be in the central cell, until the resolution corresponding to the sonic radius is reached. For adiabatic runs, this has no effect on the general aspect of the flow, since the pressure is almost uniform, in contrast to nonadiabatic runs. We present in Figure 4 the velocity, temperature, pressure, and baryon density profiles at \(z = 0\) for various mesh resolutions. It can be seen that apart from an increasing sharpness of the shock front and an increasing density contrast in the central cell, the resolution has little quantitative influence on the results. The velocity field is typical of an accreting quasi-hydrostatic flow. The usual self-similar scaling laws \(T_{\text{ad}} \propto x^{2/3}, n_{\text{ad}} \propto x^{-2/3}, \) and \(P_{\text{ad}} \approx \text{const.}\) are well reproduced.

### 3.3. Nonadiabatic Collapse

We now turn to the analysis of nonadiabatic pancake collapse, focusing on the temperature structure in the flow resulting from the microscopic collisional processes among the various species. We examine the effects of both the energy exchange processes and electronic conduction.

#### 3.3.1. No Electronic Conduction

We precisely follow chemical reactions with the corresponding thermochemistry, collisional cooling processes, and equipartition processes, as discussed in § 2. We first suppose that electronic conduction is ineffective. Figure 5 shows that the electronic temperature decouples from the ion temperature at 600 kpc \(h^{-1}\) from the midplane. The maximum departure from equilibrium is found near the shock front at 1.1 Mpc \(h^{-1}\). In this region, the ion temperature is about \(10^{7}\) K, while the electron temperature barely reaches \(10^{6}\) K. Furthermore, the ion and electron temperature profiles are different, with opposite gradients; the electron temperature steadily drops toward the front, while the ion temperature rises.

Nonequilibrium chemistry is required especially in the postshock regions, where ionization gradually reaches its near-equilibrium value. Recall that electrons are essentially heated behind the shock front by Coulomb collisions with hot ions. Since equipartition processes are conservative, the total energy density (i.e., the total pressure) is unchanged.

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**Fig. 4.**—Density, velocity, temperature, and pressure profiles at \(z = 0\) for the adiabatic collapse of the reference pancake \((L = 16 \text{ Mpc} h^{-1}, a = 0.2, \) and \(\Omega_b = 0.1)\). In each graph we plot three runs with increasing resolution (dashed line, \(N = 128\); dotted line, \(N = 256\); and solid line, \(N = 1024\)).
relative to the single-temperature case. By themselves, equipartition processes do not affect the dynamics of the flow, which is only modified (relative to the adiabatic case) by cooling. Since the equipartition rates per particle are proportional to density, the temperatures of ions and electrons are well coupled in the dense parts of the pancake, but significantly decouple in the low-density outer regions. The equilibrium point (where and differ by less than 2%) will be roughly estimated by analytical calculations presented below.

3.3.2. Electronic Conduction

In this case, we suppose that electronic conduction is fully effective, with flux-limited diffusion (Cowie & McKee 1977). We find that conduction is saturated only in the central region, where temperature gradients are very stiff, and in the outermost regions, where the density is very low. Computing thermal fluxes is a complicated task, since it depends on the ionization state of the gas, which in turn depends on the propagation speed of the ionizing thermal wave. We therefore need a good sampling of the ionization front to accurately track the thermal front. This explains why we chose a linear mesh, in order to achieve a fair sampling of temperature and abundance profiles in the thermal wave.

In Figure 6 we plot the pancake state at \( z = 0 \). Note that the ionization state of the gas is very well sampled and that abundances gradually evolve toward their equilibrium values. The shock front position at 1 Mpc \( h^{-1} \) is very close to its position in the no-conduction run. The main effect of conduction is the thermal precursor, which preheats and preionizes the gas up to 1.5 Mpc \( h^{-1} \) from the midplane. Because equipartition processes are slow in this region, the ion temperature reaches only \( 10^5 \) K, while the electron temperature is \( 10^6 \) K. Nevertheless, this results in a slight dynamical effect on the flow: ion pressure gradients cause a small deviation from the pressureless velocity profile in the unshocked region, clearly visible on this figure. Shock-heated regions occupy a total volume of 2 Mpc \( h^{-1} \), while unshocked but preheated (\( T_i \approx 10^5 \) K) and preionized (\( T_e \approx 10^6 \) K) regions occupy a total volume of 1 Mpc \( h^{-1} \). As we show in the next section, the efficiency of electronic conduction depends strongly on the pancake size.

3.4. Varying the Pancake Parameters

In this section, we study the influence of the different parameters on the pancake structure. We develop approximate formulae that guide our conclusions. We assume that, in any case, the dynamical state of the pancake is given by the adiabatic collapse. Following Bond et al. (1984) and Shapiro & Struck-Marcell (1985), it is then possible to derive interesting formulae for the pancake evolution.

We assume first that each fluid element \( q \) is shock heated at an epoch given by

\[
\frac{a_s}{a_c} = \frac{\pi q}{\sin \pi q},
\]
This corresponds to the epoch at which the corresponding collisionless particle crosses the center of the pancake. We also suppose that the gas is fully ionized and that the flow remains strictly adiabatic. Before the shock front, the flow follows the pressureless solution of pancake collapse (Zeldovich 1970). Using Rankine-Hugoniot relations and assuming that the postshock peculiar velocity vanishes, we get the postshock temperature and the postshock overdensity,

\[ kT = \frac{1}{2} \mu m_p \xi^{-1} (H_0 L)^2 a^2 \]  \hspace{1cm} (29)

\[ 1 + \delta = \frac{4}{1 - \pi q (\cos \pi q) / (\sin \pi q)} . \]  \hspace{1cm} (30)

As we assumed that the peculiar velocity is zero in the postshock region, the temperature evolves afterward as \(a^{-2}\) and the density as \(a^{-3}\). Mass conservation also implies that the Eulerian position of a given fluid element in the shocked region is given by

\[ x = \int_0^{\pi q} \left( 1 - \pi q \frac{\cos \pi q}{\sin \pi q} \right) dq . \]  \hspace{1cm} (31)

This allows us to describe the dynamical evolution (single-temperature case) of the pancake. Let us now estimate the thermodynamical evolution using our three-temperature formalism. The equipartition timescale for electron-ion energy exchange is given by

\[ t_{ei} = 503 \frac{T_{ei}^{3/2}}{n_e \ln \Lambda} \text{ s} . \]  \hspace{1cm} (32)

Assuming that the effective temperature \(T_{ei}\) is equal to the postshock adiabatic temperature, the equipartition timescale will remain constant during the postshock evolution (we neglect the slow variation of the Coulomb logarithm, taking \(\ln \Lambda \approx 40\)). It is now possible to solve analytically the equipartition equation,

\[ \frac{d}{dt} \left( T_e - T_i \right) + 2 \frac{\dot{a}}{a} (T_e - T_i) = -\frac{4}{t_{ei}} (T_e - T_i) . \]  \hspace{1cm} (33)

The single temperature, given by equation (29), is related to \(T_e\) and \(T_i\) by

\[ T = \frac{n_e T_e + n_i T_i}{n_e + n_i} . \]  \hspace{1cm} (34)

We finally obtain semianalytical temperature profiles, plotted in Figure 7, for the reference pancake at \(z = 0\). Note that numerical results qualitatively agree well with our analytical theory. Because we assume that the postshock velocity vanishes, we overestimate the shock front position and the postshock temperature. In the numerical calculation, Lagrangian fluid elements pile up deeper than we assume in our analytical calculation. This explains the visible differences between the numerical and analytical results.

The pancake structure is fully described by three characteristic points, as presented in previous sections: the compression point, where ions and neutral particles are shocked; the thermal point, marking the end of the thermal wave; and the equilibrium point, where equilibrium
Assuming that we can write increased) sufficiently.

tures appear mainly at late epochs and in the outermost for the shock front. This means that nonequilibrium fe-
dependence of the equilibrium point is much slower than 

total shock-heated mass for the case, and

mass at thermodynamical equilibrium is about 85% of the 

equilibrium point reaches much deeper regions. The Ñnal 

baryon density parameter is decreased from 0.1 to 0.01, the 

the equipartition timescale on temperature ( 

pancake size. This is because of the strong dependence of 

It appears that this coordinate depends strongly on the 

clusters, where thermodynamical equilibrium is efficiently 

mergers strongly decouple electrons and ions through 

tron pressure by up to 1 order of magnitude. This e†ect can 

outer regions of clusters can di†er from the observed elec-

This could lead to an underestimate of the cluster mass in 

regions. In the central hydrostatic part of clusters, where thermodynamical equilibrium is efficiently 

recovered, such effects are not likely to appear. We address 

this question using fully three-dimensional X-ray cluster 

modeling in a companion paper et al.(Chie ` ze 1998a)

We show that electronic conduction in the outermost 

regions, if effective, leads to a thermal wave escaping the 

shock-heated regions of the pancake. This thermal precu-

ror could have interesting cosmological consequences, such 

as late reionization and heating of noncollapsed regions. In 

our case, the precursor is strongly confined by the very high 

infall velocity toward the pancake center. In a more
complex geometry, one can imagine that the size of the precursor could be much more extended, leading to efficient heating of the intergalactic medium. This effect might be detected in the vicinity of very large X-ray clusters.

Nonequilibrium regions (from the thermal precursor to the equilibrium point) are very extended and dominate in volume the structure of pancakes (this paper) and X-ray clusters (Chièze et al. 1998a). Using high-sensitivity experiments, such as the X-ray satellite *XMM* (Fabian 1987, p. 581), we should in future be able to observe the low-density parts of clusters, where all these processes are likely to be very important.

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