

Numerical simulation of interface for compressible fluids

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Résumé — This short note describes the main difficulties encountered in the simulation of interface for compressible flows and some of the existing solutions to do it correctly. We also discuss one multiphase model.

Mots clés — compressible interface, compressible multiphase problems

We are interested in the numerical simulation of compressible flows when the fluid is made of several components or phases. Throughout the paper, we consider a fluid with two components or phases denoted by Σ_1 and Σ_2 . Each phase has its own equation of state (EOS), $p_i = p_i(\rho_i, \varepsilon_i)$ where ρ_i is the density of Σ_i and ε_i is its specific internal energy. A priori, each phase has its own temperature T_i , and $\varepsilon_i = \varepsilon_i(T_i, \rho_i)$ for example. Similarly, one can introduce the entropy and of course the EOS are thermodynamically consistent.

Two types of mixture models can be considered and they differ by the form of the equation of state.

1. In the first one, we denote then the Σ_i 's as components, the mixture obeys the Dalton's law, $p = p_1 + p_2$. This assumes that $T_1 = T_2 = T$ which means that the Σ_1 and Σ_2 are intimately mixed, and there are enough collisions between atoms so that one can define a single temperature T . This occurs in combustion problems, hypersonic flows, etc.
2. In the second one, we denote the Σ_i 's as phases which means that there is no intimate mixture between Σ_1 and Σ_2 . This situation occurs in multiphase flow situations, such as alloys (seen as compressible media), bubbly flows, etc. If one introduces α_i the volume fraction of Σ_i , we have $\alpha_1 + \alpha_2 = 1$. The pressure is then $p = \alpha_1 p_1 + \alpha_2 p_2$.

In this paper we only consider the second case even though many similarities exist between the two cases. In the second situation, the equation of state of Σ_1 and Σ_2 may be *very* different. The simplest case occurs when Σ_1 and Σ_2 obeys the stiffened gas EOS,

$$p_i = \frac{\rho_i \varepsilon_i + \gamma_i p_{i,\infty}}{\gamma_i - 1}$$

which covers the case of standard air ($\gamma = 1.4$ and $p_{i,\infty} = 0$) or more complex gases such as water, copper, etc, when one neglects the non spherical part of the Cauchy stress tensor. Much more complex case have to be dealt with, such as the EOS of the Mie-Grüneisen form,

$$p_i = P_i(\rho_i) + \rho_i \Gamma_i (\varepsilon_i - \varepsilon_i(\rho_i)) \quad (1)$$

with highly non linear functions for P_i and ε_i for which it is essential that ρ_i belongs to the range of validity of the EOS (which is in general much smaller than \mathbb{R}^+ ...).

In this paper, we focus on the Eulerian formulation of the flow equations, and assume also that the two fluids have the same velocity. For the sake of simplicity, we also assume one dimensional problems. We focus on two different, but related, cases : pure interface problems, multiphase flows. In an interface problem, the thermodynamic properties of the flow change only at the interface. In other words, there is

a curve $t \mapsto x(t)$ such that if $x < x(t)$ then the flow is Σ_1 and when $x > x(t)$ we have Σ_2 . In multiphase flows, any volume may contain both Σ_1 and Σ_2 . In pure interface problems we have $\alpha_i = 0$ or 1 at any point; in the multiphase case, we can have $\alpha_1\alpha_2 > 0$. Interface problems are in some way embedded into the set of multiphase flow problems.

1 Pure interface problems

One simple model for this situation is

$$\frac{\partial \alpha_1}{\partial t} + u \frac{\partial \alpha_1}{\partial x} = 0 \quad (2a)$$

with

$$\begin{aligned} \frac{\partial(\alpha_1 \rho_1)}{\partial t} + \frac{\partial(\alpha_1 \rho_1 u)}{\partial x} &= 0, & \frac{\partial(\alpha_2 \rho_2)}{\partial t} + \frac{\partial(\alpha_2 \rho_2 u)}{\partial x} &= 0 \\ \frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2 + p)}{\partial x} &= 0, & \frac{\partial E}{\partial t} + \frac{\partial[u(E + p)]}{\partial x} &= 0, \end{aligned} \quad (2b)$$

$E = e + \frac{1}{2}\rho u^2$, $\rho = \alpha_1 \rho_1 + \alpha_2 \rho_2$, $e = \alpha_1 e_1 + \alpha_2 e_2$. The EOS of the fluids are such that $e_i = \rho_i \varepsilon_i(\rho_i, p_i)$ and we assume pressure equilibrium. This is an hyperbolic system, see appendix A. This model has also a fully conservative version since the first equation can be replaced by

$$\frac{\partial(\alpha_1 \rho)}{\partial t} + \frac{\partial(\alpha_1 \rho u)}{\partial x} = 0 \quad (2c)$$

The solution of the Riemann problem shows that α and Y change only across the contact wave across which the pressure and the velocity remain constant. From a practical point of view, if one extends directly standard solvers using the conservative formulation (2c)-(2b), it is not possible to respect correctly the interface conditions. The scheme will converge to the correct solution, but extremely slowly, see [2, 10]. The problems comes from the fact that numerically speaking, the pressure and the velocity will not stay constant at interface. Easy counter examples can be found even for supersonic flows (where most schemes reduce to an upwind scheme), see [1]. The fundamental reason comes from the fact that the numerical dissipation occuring for each component of (2c)-(2b) is not compatible in general with the respect of interface condition. As shown in [1], this is a general drawback of conservative scheme. A solution to remedy this problem is to accept to loose full conservation. This has been first done by Karni [11] then Abgrall [2] for a mixture model, and then by Saurel & Abgrall [17] for interface problem. In these references, the equation of state is rather simple (mixture of calorically perfect gaz for the mixture models, or stiffened gas EOS for the interface models), so that the solution amounts to find a discretisation of the evolution equations of the thermodynamic parameters, these equations being another interpretation of (2a). However, in the case of more sophisticated EOS, such as Mie Grüneisen EOS, we cannot apply this method. The explanation is very simple : P_i and ε_i , the parameters in (1), depend on ρ_i which has already be computed from the approximation of (2b). This may lead to inconsistencies. To overcome this, one can use a “linearized” equivalent stiffened gas EOS as in [18] and further references by Saurel, or the ghost fluid method [3]. The original ghost fluid method [9] has some thermodynamical inconsistencies (for example, the entropy is extrapolated across an interface). In our opinion, a better method is presented in Abgrall & Karni [3] in 1D, then in 2D [12], and then improved in [8].

The idea is very simple. We explain it for first order schemes, more information can be found in [3, 8]. As usual, we consider a partition of \mathbb{R} in cells $]x_{j-1/2}, x_{j+1/2}[$, $j \in \mathbb{Z}$. To make things simpler, we assume that the cells have the same length Δx , but this assumption is not essential. We define $x_j = \frac{x_{j-1/2} + x_{j+1/2}}{2}$ the cell center. We replace (2a) by a level set equation

$$\frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} = 0$$

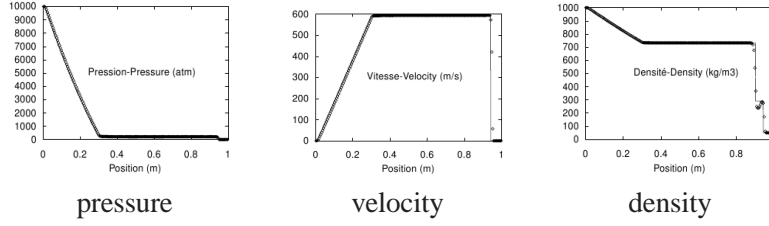


FIGURE 1 – Density, pressure, and velocity for the Riemann problem defined in table 1. 200 cells. From [13].

with f_i^0 defined as the signed distance between the initial interface and the cell center x_i . This PDE is evolved, for example, by the upwind scheme. The system (2b) is in conservation form, let us denote by $U = (\alpha_1 \rho_1, \alpha_2 \rho_2, \rho u, E)^T$ the conserved variable. A purely conservative scheme would evolve (2b) with a conservative scheme

$$U_j^{n+1} = U_j^n - \lambda (F_{j+1/2} - F_{j-1/2}), \quad \lambda = \frac{\Delta t}{\Delta x}. \quad (3)$$

The numerical flux $F_{j+1/2}$ is a function of the physical variables $W = (\alpha_1, \rho_1, \rho_2, u, p)$ and the equation of state EOS that one uses in the cells j and $j+1$, $F_{j+1/2} := F(W_j^n, W_{j+1}^n; EOS_j^n, EOS_{j+1}^n)$. If one does so, there will be pressure oscillations because of the numerical diffusion.

Over one time step, the GFMP algorithm proceeds as follows. Note that the order of the operation is essential to respect the structure of the contact :

1. Assume $(\alpha_1, \rho_1, \rho_2, u, p, f)$ are given in each grid cell j .
2. Use the level-set function f to determine the location of the material interface.
3. Compute the conserved quantities $(\alpha_1 \rho_1, \alpha_2 \rho_2, \rho u, E)$ in each cell, using the appropriate EOS as determined by the sign of f (*).
4. If $f_j \cdot f_{j+1} > 0$ then we have the same EOS in both cells. Compute the inter-cell flux $F_{j+\frac{1}{2}}(W_j, W_{j+1}; EOS_j, EOS_{j+1})$ using the EOS.
5. Otherwise compute two inter-cell fluxes at $x_{j+\frac{1}{2}}$, $F_{j+\frac{1}{2}}(W_j, W_{j+1}; EOS_j, EOS_j)$ and $F_{j+\frac{1}{2}}(W_j, W_{j+1}; EOS_{j+1}, EOS_{j+1})$
6. Update U^n following (3) with the appropriate flux defined as follows : use $F_{j+\frac{1}{2}}(W_j, W_{j+1}; EOS_j, EOS_j)$ to update U_j^n and $F_{j+\frac{1}{2}}(W_j, W_{j+1}; EOS_{j+1}, EOS_{j+1})$ to update U_{j+1}^{n+1} .
7. Compute the new primitive variables $W = (\alpha_1, \rho_1, \rho_2, u, p)$.
8. Compute the level-set function f .

We make the following observations.

- First, the algorithm is obviously not conservative, since the flux out of cell j is different from the flux into cell $j+1$. However, using the two-flux update as described above affects *only* the total energy balance, through the internal energy contribution. Mass and momentum are still perfectly conserved, see [3].
- Second, each one of the two flux formulas "sees" only *one* fluid, both in the data U_j^n and in the solution U_j^{n+1} . Contact surfaces are therefore correctly recognized, as they do in single fluids. In particular, as shown in (*) if u and p are uniform in the data, they will remain uniform in the solution, provided the numerical flux for "pure" fluids do so. This can be a tricky issue in some circumstances, see appendix B
- Third, material interfaces, like any other discontinuous fronts, are captured hence are numerically diffused. However, this does not cause spurious pressure oscillations to arise.

	ρ (Kg/m^3)	p (Pa)	u (m/s)	γ	p_∞ (Pa)
Liquid	1000	10^9	0	4.4	$6 \cdot 10^8$
Gas	50	10^5	0	1.4	0

TABLE 1 – Initial conditions for the Riemann problem represented in figure 1.

An example of application of this method, taken from [13, 5] is shown in figure 1 with 200 points. The conditions are given in table 1. Two and three dimensional applications, with some improvement are presented in [8] for underflow explosions.

2 Multiphase flows

The system is that of a two compressible phase flows Σ_1 and Σ_2 for which $\alpha_1\alpha_2$ may be strictly positive. In that case the system (2) cannot be used since it does not take into account any interaction between fluids. Imagine for example a shock wave moving in a bubbly media. According to the acoustic impedance of each phase, the bubble may expand or compress, hence the shock wave modifies the local form of the volume fraction α . These interactions are generally taken by introducing inter-facial pressure and inter-facial velocities. A good introduction of these modeling issues can be found in Drew and Passman [7], Baer and Nunziato model [6]. We follow here the approaches taken in [18], then [4] where a scheme is derived following [7], and mainly [15]. In this last reference, an asymptotic model is derived. The inverse of the small parameter can be interpreted as the inter-facial area between phases. Hence the model tends to describe the situation of a two phase flow where in any element of volume, the two phases may coexist without being mixed. This leads to a system of PDEs, satisfied by the smooth solution, where (2a) is replaced by

$$\frac{\partial \alpha_1}{\partial t} + u \cdot \nabla \alpha_1 = K \operatorname{div} u \quad (4)$$

and these other variables $(\alpha_1 \rho_1, \alpha_2 \rho_2, \rho u, E)$ (with $\alpha_2 = 1 - \alpha_1$) follow (2b). We assume velocity and pressure equilibrium. In this model, each fluid has its own equation of state. In these relations, u is the fluid velocity, $e = \varepsilon + 1/2 \rho u^2$, $\rho \varepsilon = \alpha_1 \rho_1 \varepsilon_1(p, \rho_1) + \alpha_2 \rho_2 \varepsilon_2(p, \rho_2)$, and

$$K = \frac{\rho_1 a_1^2 - \rho_2 a_2^2}{\frac{\rho_1 a_1^2}{\alpha_1} + \frac{\rho_2 a_2^2}{\alpha_2}}, \quad (5a)$$

where a_i is the speed of sound of phase Σ_i . The system (4)-(2c) is hyperbolic. The eigenvalues are u (3 times) and $u \pm a$ where a is the Wallis speed of sound defined by

$$\frac{1}{\rho a^2} = \frac{\alpha_1}{\rho_1 a_1^2} + \frac{\alpha_2}{\rho_2 a_2^2}, \quad (5b)$$

The fields associated to $u \pm a$ are genuinely non linear, the three other are linearly degenerate.

R. Saurel et al., in [20], have developed a series of shock relations for the system (4)-(2c) that write, if $Y = \rho_1 \alpha_1 / \rho$,

$$\Delta Y = 0, \quad \Delta \varepsilon_1 + \bar{p} \Delta \tau_1 = 0, \quad \Delta \varepsilon_2 + \bar{p} \Delta \tau_2 = 0,$$

with $\bar{p} = \frac{p_L + p_R}{2}$ and $\Delta f = f_L - f_R$. These jump relations enable to solve the Riemann problem, note that they are completed with the standard jump relation on the linear wave.

Computing the solutions of (4)-(2c) even in the case of discontinuous solutions is a very complex task because of (4). In a sequence of papers, Saurel and co-authors [16, 19, 21] have devised several methods for computing this, however the methods appear quite complex. The reason of the numerical

	α	p (Pa)	u (m/s)	ρ_1 (Kg/m ³)	ρ_2 (Kg/m ³)	Fluid	p_∞	γ
Σ_1	0.5954	$2 \cdot 10^{11}$	0	1185	3622	Σ_1	$5.3 \cdot 10^9$	2.43
Σ_2	0.5954	10^5	0	1185	3622	Σ_2	$1.41 \cdot 10^{11}$	1.62

TABLE 2 – Conditions for the 5 equations model.

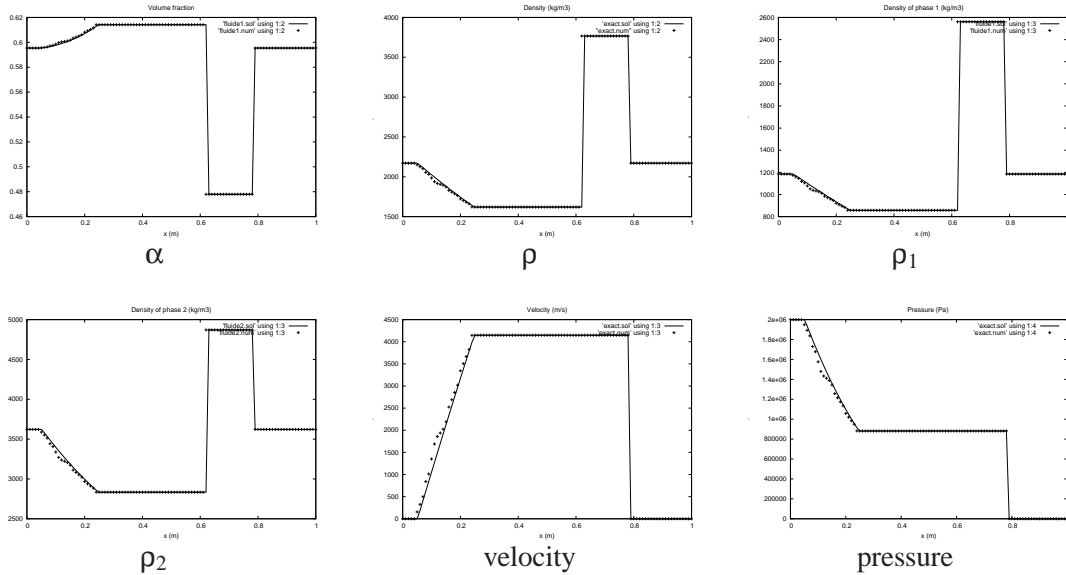


FIGURE 2 – Solution for the conditions of table 2.

difficulties comes from the fact that one has to accurately represent the thermodynamic path that links the left and right states of shocks. Up to our knowledge, there is *no* finite difference/finite volume like scheme that permit to compute the solution of this system without any parameter tuning. The reason lies in the numerical dissipation of the schemes which mimic a thermodynamic path that is not correct. For conservative systems, the thermodynamics path is not correct either, but thanks to the Lax Wendroff theorem, the solution will converge correctly if enough entropy inequalities are satisfied.

To our best knowledge, the only way to possibly compute the correct solutions is to use a method that is dissipation free. There are two such methods : the Random Choice Method and front tracking. We apply the RCM method on that system without any modification. The initial conditions and the EOS parameters are given on table 2. The mesh has 100 grid points, the CFL number is set to 0.5 and the final time to $t = 29 \cdot 10^{-6}$ s. The solution is displayed on Figure 2 and is in excellent agreement with the exact solution, especially for the shock capturing properties.

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A Derivation of the eigenvalues of the interface model.

The simplest is to rewrite the system (2) in term of $\alpha := \alpha_1, Y_1, \rho, u$ and p . we have introduced the mass fraction $Y := Y_1 = \alpha_1 \rho_1 / \rho$. The system (2) is transformed into

$$\frac{\partial \alpha}{\partial t} + u \frac{\partial \alpha}{\partial x} = 0, \quad \frac{\partial Y}{\partial t} + u \frac{\partial Y}{\partial x} = 0, \quad \frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} + \rho \frac{\partial u}{\partial x} = 0, \quad \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \frac{1}{\rho} \frac{\partial p}{\partial x} = 0, \quad \frac{\partial e}{\partial t} + (e+p) \frac{\partial u}{\partial x} + u \frac{\partial e}{\partial x} = 0 \quad (6)$$

Then we need to write the derivative of e in term of these variables. Using $e = \alpha_1 e_1 + \alpha_2 e_2, Y_1 + Y_2 = 1$ and $\alpha_1 + \alpha_2 = 1$, and differencing, we get :

$$\begin{aligned} de &= \left(\alpha_1 \frac{\partial e_1}{\partial p_1} + \alpha_2 \frac{\partial e_2}{\partial p_2} \right) dp + \left(Y_1 \frac{\partial e_1}{\partial \rho_1} + Y_2 \frac{\partial e_2}{\partial \rho_2} \right) d\rho + \left(\rho_1 \frac{\partial e_1}{\partial \rho_1} - \rho_2 \frac{\partial e_2}{\partial \rho_2} \right) dY + \left(\rho_1 \frac{\partial e_1}{\partial \rho_1} - \rho_2 \frac{\partial e_2}{\partial \rho_2} + e_1 - e_2 \right) d\alpha \\ &:= Edp + Cd\rho + BdY + Ad\alpha \end{aligned}$$

Using this and (6), we can eliminate $\frac{\partial e}{\partial t}$ and $\frac{\partial e}{\partial x}$, and we get

$$\begin{aligned} \frac{\partial \alpha}{\partial t} + u \frac{\partial \alpha}{\partial x} &= 0, & \frac{\partial Y}{\partial t} + u \frac{\partial Y}{\partial x} &= 0 \\ \frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} + \rho \frac{\partial u}{\partial x} &= 0, & \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \frac{1}{\rho} \frac{\partial p}{\partial x} &= 0 \\ \frac{\partial p}{\partial t} + K \frac{\partial u}{\partial x} + u \frac{\partial p}{\partial x} &= 0 \end{aligned} \quad (7)$$

with $K := \rho \frac{h-C}{E}$, where $h = (e+p)/\rho$ is the specific enthalpy. The eigenvalues of the Jacobian matrix of (7) are $\lambda = u$ 3 times, $u \pm c$ with

$$c^2 = \frac{h-E}{C}.$$

We can rewrite this in a maybe more familiar way. Introducing $\kappa = 1/E, \chi = -C/E, \nu = A/E$ and $\mu = A/E$, we have $dp = \kappa de + \chi d\rho + \nu d\alpha + \mu dY$ and the square of the speed of sound is

$$c^2 = \kappa h + \chi.$$

The parameter κ is identical to $\gamma - 1$ for a perfect gas. We note that for a thermally consistent fluid, $\frac{\partial e_i}{\partial p_i} \geq 0$ and $\frac{\partial e_i}{\partial \rho_i} \geq 0$, so that κ and χ are both positive. We can easily show that the Jacobian matrix admits a complete set of eigenvectors, namely

- Associated to $\lambda = u$: $r_1 = (1, 0, 0, 0, 0)^T, r_2 = (0, 1, 0, 0, 0)^T, r_3 = (0, 0, 1, 0, 0)^T$
- Associated to $\lambda = u \pm c$: $r_4 = (0, 0, \rho, c, \rho c^2)^T, r_5 = (0, 0, \rho, -c, \rho c^2)^T$

Hence the system is hyperbolic. Any vector $U = (A_1, A_2, A_3, A_4, A_5)^T$ can be decomposed on the eigenbasis, $U = \sum_i \alpha_i r_i$,

$$\alpha_1 = A, \alpha_2 = B, \alpha_3 = A_3 - \frac{A_4}{c^2}, \alpha_4 = \frac{1}{2} \left(\frac{E}{\rho c^2} + \frac{D}{c} \right), \alpha_5 = \frac{1}{2} \left(\frac{E}{\rho c^2} - \frac{D}{c} \right).$$

This shows that in fans, α_i and Y_i remain constant and the standard relations

$$\frac{dp}{d\rho} = c^2, \quad \frac{dp}{du} = \mp \rho c.$$

The first relation is nothing more than $ds = 0$.

In discontinuities, we consider the model (2c)-(2b). Hence, we get the jump relations, setting $v = u - \sigma$ where σ is the velocity of the discontinuity ($H = h + v^2/2$), $[\rho_i \alpha_i v] = 0, [\rho v^2 + p] = 0, [\rho v H] = 0$. The discussion is very standard.

- Contact : If $v_L = v_R = 0$, then $[p] = 0$ and the other variables are arbitrary. In particular $[\rho_i \alpha_i]$ is arbitrary as well as $[Y_i]$, so that $[\alpha_i]$ is also arbitrary.
- Shock : if $[v] \neq 0$. We set for any variable w , $\bar{w} = (w_L + w_R)/2$. Then the mass relations give, since $\rho_i \alpha_i = Y_i \rho$,

$$[\rho_i \alpha_i v] = [\rho Y_i v] = \bar{\rho v} [Y_i] + \bar{Y}_i [\rho v] = \bar{\rho v} [Y_i] = 0.$$

Since $\bar{\rho v} = \rho_L v_L = \rho_R v_R \neq 0$, we have $[Y_i] = 0$. The relation (2c) gives $[\rho \alpha_i v] = \bar{\rho v} [\alpha_i] + \bar{\alpha}_i [\rho v] = \bar{\rho v} [\alpha_i] = 0$. Since $\bar{\rho v} \neq 0$, we get $[\alpha_i] = 0$. This shows that we have the standard shock relations and conservation of Y_i and α_i .

B Respect contacts in pure fluids.

To illustrate the problem, we consider Godunov's scheme and fluids with a calorically perfect EOS, with constant γ . One of the properties of the Godunov scheme (which is shared by the Roe scheme too) is the following. Assume that $u_i^n = u$ and $p_i^n = p$, then $u_i^{n+1} = u$ and $p_i^{n+1} = p$. This means that a contact stays numerically a contact. Let us consider the cell C_i . We have $u_{i-1}^n = u_i^n = u_{i+1}^n$ and $p_{i-1}^n = p_i^n = p_{i+1}^n$. We assume $u > 0$ for the sake of simplicity. At the interfaces $x_{i\pm 1/2}$, the solution of the Riemann problems are just contact discontinuities. Hence the numerical flux $F_{i-1/2}$ is $F_{i-1/2} = (\rho_{i-1}^n u, \rho_{i-1}^n u^2 + p, u(E_{i-1} + p))^T$. From this we get

$$\begin{pmatrix} \rho_i^{n+1} \\ \rho_i^{n+1} u_i^{n+1} \\ E_i^{n+1} \end{pmatrix} = \begin{pmatrix} \rho_i^n \\ \rho_i^n u_i^n \\ E_i^n \end{pmatrix} - \lambda \begin{pmatrix} u(\rho_i^n - \rho_{i-1}^n) \\ u^2(\rho_i^n - \rho_{i-1}^n) \\ u(E_i^n - E_{i-1}^n) \end{pmatrix}.$$

From this we see that $u_i^{n+1} = u_i^n$ and since

$$E_i^n - E_{i-1}^n = \left(\frac{p}{\gamma-1} + \frac{1}{2} \rho_i^n u^2 \right) - \left(\frac{p}{\gamma-1} + \frac{1}{2} \rho_{i-1}^n u^2 \right) + \frac{1}{2} u^2 (\rho_i^n - \rho_{i-1}^n) \quad (8)$$

By combining (8) with the total energy evolution, we see that $p_i^{n+1} = p$.

Remark B.1. *This proof uses the structure of the equation of state. Of course, it is possible to define the solution of the Riemann problem for more general equations of state, see for example [14] for a very interesting discussion. The definition of the Godunov scheme does not make use of the structure of the EOS, but is a general technique. It can easily be shown that all the previous properties go through, except the one on the contact discontinuity. The fundamental reason is the structure of the EOS, see [16]. If in general, we get $u_i^{n+1} = u$, because one only uses the fact that the pressure is uniform, the energy evolution equation becomes (using $u_i^{n+1} = u$)*

$$e(\rho_i^{n+1}, p_i^{n+1}) = e(\rho_i^n, p_i^n) - \lambda u \left(e(\rho_i^n, p_i^n) - e(\rho_{i-1}^n, p_{i-1}^n) \right),$$

and we see that there is no reason, in general, that $p_i^{n+1} = p$. . . This is a big problem since the Godunov scheme is in a way the best solver because the closer from the true Riemann problem.