Simulating interfaces in two-phase flows

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1 Introduction.

We discuss the modelling and numerical aspects of the direct numerical simulation of compressible two-phase flows, i.e. including material interfaces. Modelization and simulation of bifluid and diphasic flows have become of increasing interest among the computational fluid dynamic community. So-called direct simulation, on the contrary of average models, involves the description of the interface between fluids which is a discontinuity surface for the material properties. The modelling of multifluid flows with interfaces (i.e. immiscible components without phase change) is classical, and many numerical methods are available (such as volume of fluid (VOF), front-tracking, or level set), see e.g. [5], [13], [14], [21]. However, if phase change is taken into account at the interface, modelling is still an issue. In an incompressible setting Juric and Tryggvason proposed to consider the interface as a sharp material discontinuity and add a non-equilibrium Clapeyron-type equation to determine the interface velocity [9], [23]. In a compressible setting the well-known Korteweg-Van Der Waals theory of capilarity (also known as the second gradient theory) allows to model the phase change as a continuous process taking place in a thick transition layer (which can be seen as a diffused interface). This has been used recently by Jamet for numerical simulations [8]. Somehow our approach lies in between these two previous ones. We decide to model the phase interface as a sharp discontinuity but the supplementary equation which gives the interface velocity is now deduced from an asymptotic process performed on an underlying microscopic Korteweg-Van Der Waals model.

In the first part of this paper we address this modelling issue. Following the lead of [1], [20], [22] (among others) we derive a so-called kinetic relation which gives the mass flux at the phase interface. In a second part we introduce mixing rules for the two phases since any eulerian scheme will necessary spread out the interface and one has to handle cells containing both fluids. In a third part we briefly describe our numerical algorithm and present some computational results. We choose an eulerian approach since lagrangian methods, such as front-tracking, although precise, are very complex to implement. The dynamical aspect of the problem is handled by the compressible Euler equations solved with a Roe scheme. An extra equation is added to the Euler system in order to advect values of a color function ψ indicating the localization of each phase. This allows to deal easily with 2-D or 3-D problems, including complex topology changes of the interface. On the other hand, it involves a lack of accuracy in the precise location of the interface. In fact, numerical diffusion tends to thicken the interface into a transition zone which is no longer a sharp discontinuity between the media. To sharpen the transition front, we discuss the use a level-set approach (introduced by Osher and Sethian in [15]) and regularization by adding non-linear source terms into the advection equations.

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2 Modelling of the two-phase flow.

We consider the motion of two compressible phases separated by a sharp interface. On the contrary of the Korteweg theory of phase transition (also called second gradient theory), our model assumes that there is no transition layer between the two phases corresponding to a spinodal zone of a global state law for the single fluid to which both phases belong. This approach has at least two advantages: first, when there is no phase transition it reduces to the classical approach for immiscible fluids, second it avoids the detailed knowledge of the physical properties of this transition layer. We shall however need an additional jump relation at the interface to close the system in case of phase change: this is the so-called kinetic relation [1], [22]. Of course this model contains less physics than the full Kortweg theory, but the former is numerically more tractable than the latter which requires a very fine discretization (since, away from the triple point, the thickness of the transition layer is very small) or an artificial thickening (for details see [8]).

To explain the structure of our model, in a first step we neglect all source terms and diffusive terms to concentrate on the resulting system of first order hyperbolic conservation laws. For each phase $i = 1, 2$, denoting by $\rho_i, u_i, p_i, \varepsilon_i, e_i$ its density, velocity, pressure, specific total energy, and internal energy, the equations away from the interface are

$$\begin{cases} \partial_t \rho_i + \operatorname{div}(\rho_i u_i) = 0 \\ \partial_t(\rho_i u_i) + \operatorname{div}(\rho_i u_i \otimes u_i + p_i I) = 0 \\ \partial_t(\rho_i \varepsilon_i) + \operatorname{div}((\rho_i \varepsilon_i + p_i) u_i) = 0 \end{cases} \tag{1}$$

with $\varepsilon_i = e_i + |u_i|^2/2$, $p_i = p_i(\rho_i, e_i)$, and supplemented with the following entropy condition

$$\partial_t(\rho_i s_i) + \operatorname{div}(\rho_i s_i u_i) \le 0.$$

At the interface, denoting by n its oriented unit normal and by σ its normal velocity, we have the following jump conditions

$$\begin{cases} [\rho]\sigma = [\rho u] \cdot n \\ [\rho u]\sigma = [\rho u \otimes u + pI] n \\ [\rho\varepsilon]\sigma = [(\rho\varepsilon + p)u] \cdot n \end{cases} \tag{2}$$

where $[f]$ is the jump across the interface of the quantity f. To close the system another relationship is required to compute the interface velocity σ. Following the works of [1], [20], [22] (and others, see references therein), this additional equation is called the kinetic relation: it gives the mass transfer at the interface $j = \rho(u \cdot n - \sigma)$ as a function of the entropy jump

$$j[s] = R(j) \le 0.$$

We explain below how the function $R(j)$ is constructed.

We now write a global model for the bulk fluid made by the juxtaposition of its two phases. Introducing a "color function" $\chi(x)$ which is the characteristic function of phase 1, we define global variables

$$\rho = \chi\rho_1 + (1-\chi)\rho_2, \;\; e = \chi e_1 + (1-\chi)e_2, \;\; p = \chi p_1 + (1-\chi)p_2, \;\; u = \chi u_1 + (1-\chi)u_2.$$

Our model is thus

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho u) = 0 \\ \partial_t(\rho u) + \operatorname{div}(\rho u \otimes u + pI) = 0 \\ \partial_t(\rho\varepsilon) + \operatorname{div}((\rho\varepsilon + p)u) = 0 \end{cases} \tag{3}$$

which, in its weak form or variational formulation, includes the jump conditions at the interface. Furthermore, the color function is advected by

$$\partial_t \chi + \left(u + \frac{j}{\rho} n \right) \nabla \chi = 0$$

where n is an extension of the interface normal throughout the domain, and j is given by the kinetic relation.

3 Kinetic relation.

To explain how to obtain a kinetic relation, we simplify our setting by considering only 1-D isothermal phase transitions (the general case is more complex but fully understood also). Following the lines of [20] and [22], we regularize our first-order isothermal system by adding viscosity and capillarity effects. We also extend the phases state laws into a single state law for the global fluid as a van der Waals state law with a spinodal zone for two-phase mixtures (see figure 1).

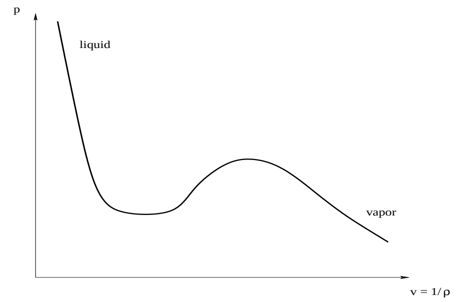

Figure 1: van der Waals type state law

The regularized system is thus

$$\begin{cases} \partial_t \rho + \partial_x (\rho u) = 0 \\ \partial_t (\rho u) + \partial_x \left(\rho u^2 + p \right) = \nu \partial_{xx} u - c \partial_{xxx} v \end{cases} \tag{4}$$

where $v = \rho^{-1}$ and ν, c are positive constants. We scale these coefficients as

$$\nu = \nu_0 \varepsilon, \;\; c = c_0 \varepsilon^2,$$

where ε is a small parameter intended to go to 0, nd we look for travelling wave solutions of the type

$$\rho \left(\frac{x - \sigma t}{\varepsilon} \right), \;\; u \left(\frac{x - \sigma t}{\varepsilon} \right),$$

with $\lim_{\xi \to \pm\infty} (\rho, u)(\xi) = (\rho^\pm, u^\pm)$. This system reduces to a single ordinary differential equation with respect to $v(\xi)$

$$-c_0 v'' + j \nu_0 v' - p(v) - j^2 v = \pi \tag{5}$$

with $j = \rho^+(u^+ - \sigma) = \rho^-(u^- - \sigma)$ and $-\pi = p(v^+) + j^2 v^+ = p(v^-) + j^2 v^-$. Multiplying (5) by v' and integrating yields

$$\int_{v^-}^{v^+} p(v) dv - \frac{p(v^+) + p(v^-)}{2} (v^+ - v^-) = \nu_0 j \int_{-\infty}^{+\infty} v'(\xi)^2 d\xi. \tag{6}$$

After some algebra, one deduces from (6) the following kinetic relation in terms of the mathematical entropy for (4) (which turns out to be the total energy $E = 1/2u^2 - \int p(v)dv$)

$$[jE + pu] = -\nu_0 j^2 \int_{-\infty}^{+\infty} v'(\xi)^2 d\xi \leq 0. \tag{7}$$

Remark that if $\nu_0 = 0$, i.e. if the phase transition is non-dissipative, (6) reduces to the well-known generalized Maxwell equal-area rule. For some simple state laws the evaluation of the integral of $v'(\xi)^2$ is explicit. More generally, one can just perform a Taylor expansion for small values of j. In any case (7) provides a supplementary jump condition at the interface which yields the value of j.

4 Modelling of the mixture layer.

From a numerical point of view we want to use an Eulerian scheme. In other words, we discretize the equations of motion on a fixed mesh, and the interface is captured, rather than tracked, on this Eulerian mesh. As for any front-capturing method, our numerical method has a tendency to diffuse the interface. In other words, instead of computing a sharp interface, we obtain a small layer of cells around the true interface in which we have a mixture of both fluids. The width of this transition layer will be controled by some anti-diffusive process as described in a next section. Although this transition layer has no special physical meaning, we have to model it in order to globally compute the hydrodynamics of the two phases in the whole domain. The purpose of this section is to present our choice of model for the two-phase mixture. We start with the simple isothermal mixing model of perfect gases, as described in [2].

Let us denote by c_{pi}, c_{vi}, respectively the specific heat at constant volume and pressure of the i^{th} fluid. If we denote by T_i its temperature, we have

$$p_i = (\gamma_i - 1)\rho_i e_i \quad , \quad e_i = c_{vi} T_i.$$

During the computation, there will be cells containing both fluids, and we need to define a new equation of state for this mixture if we want to treat it as a single equivalent fluid. This is a purely numerical artefact and we emphasize that it has no real physical meaning. We make the assumption of a thermal equilibrum, i.e. in the area where both species are present, they share the same temperature T. Furthermore, we also make the assumption that the pressure is given by Dalton's law.

Let $\rho = \rho_1 + \rho_2$ be the density of the mixture and $c_i = \rho_i/\rho$ the mass fraction of the i^{th} gas. If we note e, and p, respectively the specific internal energy and the pressure of the mixture, altogether our assumptions imply

$$\rho e = \rho_1 e_1 + \rho_2 e_2, \quad p = p_1 + p_2. \tag{8}$$

Introducing thermodynamic parameters for the mixture

$$\begin{aligned} c_p &= c_1 c_{p1} + c_2 c_{p2}, && (9)\\ c_v &= c_1 c_{v1} + c_2 c_{v2}, && (10)\\ \gamma &= \frac{c_1 c_{p1} + c_2 c_{p2}}{c_1 c_{v1} + c_2 c_{v2}}, && (11) \end{aligned}$$

those values allow us to rewrite (8) as

$$e = c_v T, \quad p = (\gamma - 1)\rho e. \tag{12}$$

Therefore, the mixture state equation is similar to that of a perfect gas, except that the γ parameter depends on the mass fractions. This mixing process can be applied to wider classes of gas, e.g. stiffened gas [17]. There are other possible mixing laws which allow to define a state equation for the mixture (see e.g. the work of Desrprés and Lagoutière). However, for real gas it is easier to drop one algebraic requirement on the mixture and to introduce a supplementary transport equation. Specifically, in [3], we drop the isothermal assumption which is replaced by a phase mass conservation. In any case, the purpose of our modelization is to view the mixture zone (as well as the entire domain) as occupied by a single equivalent fluid.

5 Numerical method.

For simplicity, we consider (3) in 1-D

$$\partial_t U + \partial_x F(U) = 0 \tag{13}$$

with

$$U = \begin{pmatrix} \rho_1 \\ \rho_2 \\ \rho u \\ \rho e \end{pmatrix}, \qquad F(U) = \begin{pmatrix} \rho_1 u \\ \rho_2 u \\ \rho u^2 + p \\ (\rho e + p)u \end{pmatrix} \quad . \tag{14}$$

This system is discretized in the following way

$$U_i^{n+1} = U_i^n - \frac{\Delta t}{\Delta x}\left[\phi_{i+1/2}^n - \phi_{i-1/2}^n\right] \tag{15}$$

where $\phi_{i+1/2}^n$ is the numerical flux at time t_n, at the interface $(i+1/2)$ which separates the cell i and the cell $(i+1)$. We use the Roe scheme [16] to solve the system. Thus the numerical flow $\phi_{i+1/2}^n$ is now expressed $\phi(U_i^n, U_{i+1}^n)$ where, considering 2 states U_L and U_R, we have

$$\phi(U_L, U_R) = \frac{1}{2}\Big[F(U_L) + F(U_R) - |A(U_L, U_R)|(U_R - U_L)\Big] \tag{16}$$

F is given by (14), and A is a matrix called Roe Matrix which depends on the states U_L and U_R. Let us recall that given a diagonalisable matrix M, given $(\lambda_i)_{i=1,N}$ and $(\vec{r}_i)_{i=1,N}$ respectively the set of its real eigenvalues and eigenvectors, we denote by R the matrix of columns $(\vec{r}_i)_{i=1,N}$, by $|\Lambda|$ the diagonal matrix of elements $|\lambda_i|$, and by $|M|$ the matrix $|M| = R|\Lambda|R^{-1}$. According to [16]

$$A(U_L, U_R) = \mathrm{d}F(U^*)$$

where F is given by (14), $\mathrm{d}F$ stands for its Jacobian, and U^* is some "average state" depending on U_L and U_R which must verify

$$F(U_R) - F(U_L) = \mathrm{d}F(U^*)(U_R - U_L).$$

In [2] a suitable average state U^* has been found. Unfortunately, this numerical scheme generates some oscillations in pressure near the contact discontinuities. Following [2] and [11] we modify the scheme in order to preserve contact discontinuities. It means that if at time t_n, there is a real contact discontinuity between two state U_L^n and U_R^n, i.e. $p_L^n = p_R^n$ and $u_L^n = u_R^n$, then at time t_{n+1} we still have a contact discontinuity between U_L^{n+1} and U_R^{n+1}: $p_L^{n+1} = p_R^{n+1}$ and $u_L^{n+1} = u_R^{n+1}$. Introducing the notation

$$\kappa = \gamma - 1 \text{ and } \xi = \frac{1}{\kappa}, \tag{17}$$

Abgrall has shown that the parameter γ must be discretized through the following relation

$$\xi_i^{n+1} = \xi_i^n - \frac{\Delta t}{2\Delta x}\Big(u_i^n[\xi_{i+1}^n - \xi_{i-1}^n] - |u_i^n|\,[\xi_{i+1}^n - \xi_{i-1}^n]\Big) \tag{18}$$

Indeed this equation is the discretization of the advection equation that ξ must verify

$$\frac{\partial \xi}{\partial t} + \vec{u}\cdot\overrightarrow{\mathrm{grad}}\xi = 0 \tag{19}$$

Finally, a convenient way to gain second order accuracy in space, consists in applying a MUSCL method to our present scheme (for details see e.g. [6]).

So far, our numerical scheme describes the interface $\Gamma(t)$ as a thick zone as does the VOF method. In order to accurately localize the interface we implement an extra step using the level set method. The main idea (see e.g. [19]) is to introduce a function $\varphi(x,t)$ such that its zero level set is precisely the interface, *i.e.*$\varphi(x,t)=0 \Longleftrightarrow x\in\Gamma(t)$. Differentiating this equation and extending it to the whole domain yields a simple transport equation for the level set function φ

$$\begin{cases} \varphi(x,0)=0 \Longleftrightarrow x\in\Gamma(0) \\ \frac{\partial\varphi}{\partial t}+\vec{u}\cdot\overrightarrow{\mathrm{grad}}\varphi=0 \qquad \forall t>0 \end{cases} \tag{20}$$

Given $\Gamma(0)$, the interface at $t=0$, a common choice for the initialization $\varphi(\cdot,0)$ of the level set function is the signed distance to the interface, *i.e.*

$$\varphi(0,x)=\begin{cases} +\mathrm{d}(x,\Gamma(0)) & \text{if } x \text{ is in fluid 2} \\ -\mathrm{d}(x,\Gamma(0)) & \text{if } x \text{ is in fluid 1} \end{cases} \tag{21}$$

Unfortunately, throughout the motion, φ is numerically updated by (20), and it does not stay the signed distance function to the interface $\Gamma(t)$. Because of numerical diffusion, the slope of φ has a tendency to flatten, and the localization of its zero level set becomes increasingly unstable. An efficient remedy is to frequently re-initialize φ without changing its zero level set, i.e. to straighten out its front without moving the interface. This can be done [21] without knowing explicitly the position of the interface, simply by solving the following Hamilton-Jacobi equation

$$\begin{cases} \frac{\partial\psi}{\partial s}(x,s)=\mathrm{sign}(\psi_0)(1-|\overrightarrow{\mathrm{grad}}\psi|) \qquad \forall s>0 \\ \psi(x,0)=\psi_0(x)=\varphi(x,t_0) \end{cases} \tag{22}$$

which is known, as s goes to infinity, to admit a steady state solution which is again the signed distance function to the zero-level set of the initial condition $\varphi(x,t_0)$ (recall that the distance function $\mathrm{d}(x,\Gamma)$ satisfies $|\overrightarrow{\mathrm{grad}}(\mathrm{d})(x)|=1$). Here s can be seen as an "evolution variable" which has nothing to do with the time variable t. Thus, solving (22) is just a convenient anti-diffusion procedure for the level set function which does not change the interface position.

In practice, instead of solving (19) we solve (20) which is equivalent upon recognizing that

$$\xi(x,t)=(\xi_2-\xi_1)H(\varphi(x,t))+\xi_1, \tag{23}$$

where H is the Heavyside function (which is 0 on negative values and 1 on positive ones). Since the Heavyside function H is not continuous, we approximate it by a smooth function H_ε such as $H_\varepsilon(d)=(1+d(d^2+\varepsilon^2)^{-1/2})/2$. It allows to compute ξ in terms of φ with a transition layer of width of order ε. If numerical diffusion spreads too much this layer, the level set φ is reinitialized by solving (22) up to steady state. This process is made every k time steps, the smaller k the faster the convergence in (22) (usually we take $k=1$). Remark that it does not require the explicit knowledge of the interface localization and is therefore not too time consuming. A simpler alternative to this level set method is to solve the advection equation (19) for ξ with an anti-diffusive non-linear source term (see [12] for details).

6 Numerical results

6.1 Shock tube

Our first test case is a bifluid shock tube described in section 6.1 of [18]. The computation is one dimensional, and at the initial time the left part of the tube contains water under high pressure ($10^9 Pa$), while the right side of the tube is filled with air at atmospheric pressure. Since the ratio between the two fluid densities is larger than 20, it allows to test the robustness of the numerical scheme. A second order scheme (with the MUSCL technique) is used. We can check that the oscillations have been successfully removed from the pressure.

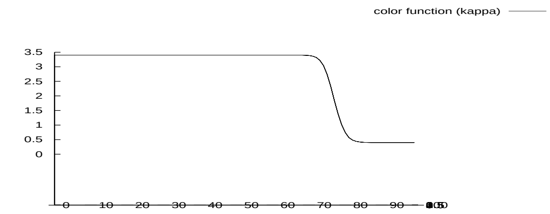

Figure 2: color function κ at $t = 2.4 \times 10^{-4} s$.

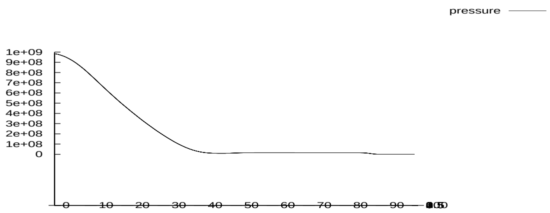

Figure 3: pressure at $t = 2.4 \times 10^{-4} s$.

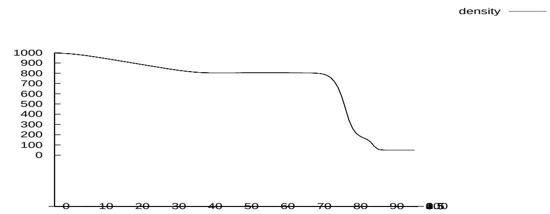

Figure 4: density at $t = 2.4 \times 10^{-4} s$.

6.2 Rayleigh-Taylor instability.

The second test case is a Rayleigh-Taylor instability between helium and air, both described as perfect gas. The computing is led on a 50×150 mesh the width-height ratio being $1/12$. Initial conditions are in the present case pressure equilibrium and a density ratio taken equal to 4.

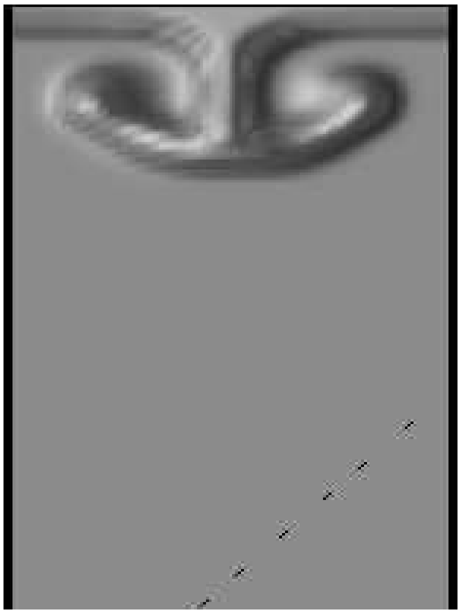

Figure 5: graph for κ at time $t = 28s$.

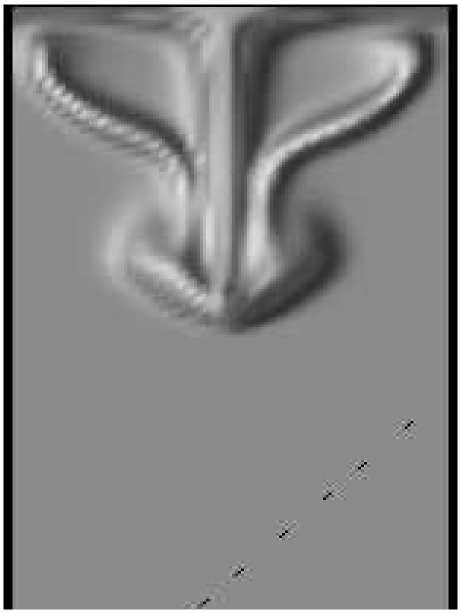

Figure 6: graph for κ at time $t = 42s$.

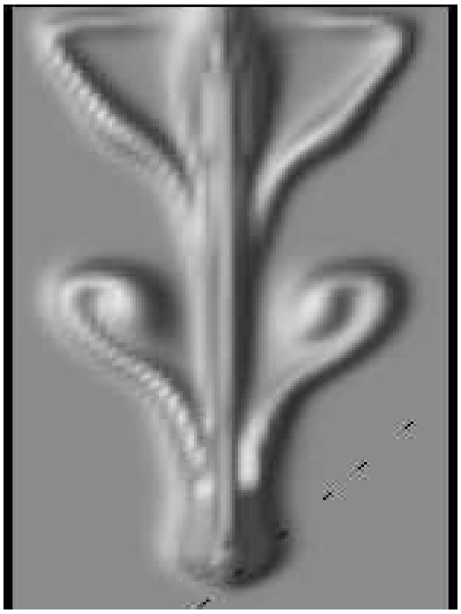

Figure 7: graph for κ at time $t = 56s$.

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