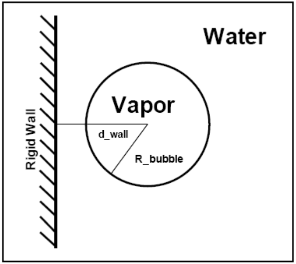
Comparison of several numerical methods for the computation of a liquid-bubble interaction

P. Helluy [a], S. Müller [b]

[a] ULP/IRMA Strasbourg, [b] RWTH Aachen

January 11, 2007

Bubble collapse



$R_{bubble} = 1$ mm
$d_{wall} = 1.5$ mm

$$p_{Water} = 5 \times 10^7 \text{ Pa}$$
$$p_{Bubble} = 2118 \text{ Pa} \tag{1}$$

A simple isothermal two-fluid model

We first study a simple barotrope isothermal two-fluid model, which is not realistic, but simpler than a model with energy.

Front capturing model

- We are interested in the flow of a compressible medium made of two fluids: a gas (1)="Air"=(A) and a liquid (2)="Water"=(W).
- The fluids are located thanks to the *gas fraction* $\varphi(x,t)$, depending on the space variable x and the time variable t.
- The fraction $\varphi = 0$ in the fluid (2) and $\varphi = 1$ in the fluid (1).

The isothermal model reads, in 1D

$$\begin{aligned} &\rho_t + (\rho u)_x = 0, \\ &(\rho u)_t + (\rho u^2 + p)_x = 0, \\ &(\rho\varphi)_t + (\rho\varphi u)_x = 0, \\ &p = p(\rho, \varphi), \end{aligned} \tag{2}$$

with the density ρ, the velocity u and the pressure p. The last conservation law is equivalent to

$$\varphi_t + u\varphi_x = 0 \tag{3}$$

because φ jumps only in contacts.

"Linear" pressure law

A possible pressure law is

$$p = p_0 + c^2(\rho - (\varphi\rho_A + (1-\varphi)\rho_W)). \tag{4}$$

where p_0 is a reference pressure, c the sound speed (the same for the two fluids) and ρ_A and ρ_W reference densities for the Air and the Water respectively.

$$\begin{aligned} \varphi = 0 \Rightarrow p = p_2 = p_0 + c^2(\rho - \rho_W), \\ \varphi = 1 \Rightarrow p = p_1 = p_0 + c^2(\rho - \rho_A). \end{aligned} \tag{5}$$

- If $\varphi \in \{0, 1\}$ at the initial time, it remains true later.
- Thus the pressure law can be modified in the mixture zone $0 < \varphi < 1$ without modifying the solution.
- However a modification has a crucial importance for the numerics.
- The isobaric modification plays a particular role: it permits to build conservative schemes that preserve constant velocity-pressure states.

Isobaric pressure law

We define the volume fraction α and the partial densities ρ_i by

$$\rho = \alpha\rho_1 + (1-\alpha)\rho_2. \tag{6}$$

The fraction is now the mass fraction is

$$\varphi = \frac{\alpha\rho_1}{\rho}. \tag{7}$$

The pressure law of each pure fluid (i) is noted p_i. We then eliminate the volume fraction by setting

$$\begin{aligned} & p = p_1(\rho_1) = p_2(\rho_2), \\ \text{or } & p = p_1\left(\frac{\rho\varphi}{\alpha}\right) = p_2\left(\frac{\rho(1-\varphi)}{1-\alpha}\right). \end{aligned} \tag{8}$$

The isobaric pressure is

$$p = p_1 = p_2 = \alpha p_1 + (1-\alpha)p_2. \tag{9}$$

We have here

$$
\begin{aligned}
p_1(\rho_1) &= p_0 + c^2(\rho_1 - \rho_A), \\
p_2(\rho_2) &= p_0 + c^2(\rho_2 - \rho_W), \\
p(\rho) &= \alpha p_1(\frac{\varphi\rho}{\alpha}) + (1-\alpha) p_2(\frac{(1-\varphi)\rho}{1-\alpha}), \\
\text{with } \alpha \text{ such that } & p_1(\frac{\varphi\rho}{\alpha}) = p_2(\frac{(1-\varphi)\rho}{1-\alpha}).
\end{aligned}
\tag{10}
$$

If ρ is fixed, $\alpha = \alpha(\varphi)$. We define

$$\theta = \frac{\rho_W - \rho_A}{\rho} > 0 \tag{11}$$

and we find

$$\alpha(\varphi) = \frac{\theta - 1 + \sqrt{(\theta - 1)^2 + 4\theta\varphi}}{2\theta}. \tag{12}$$

We can check that

$$\begin{aligned} &0 \leqslant \alpha(\varphi) \leqslant 1 \text{ if } 0 \leqslant \varphi \leqslant 1, \\ &\alpha(1) = 1, \\ &\alpha(0) = \begin{cases} 0 & \text{if} \quad \theta < 1, \\ \frac{\theta-1}{\theta} & \text{if} \quad \theta \geqslant 1. \end{cases} \end{aligned} \tag{13}$$

Thus, when the gas mass fraction is $\varphi = 0$, we have

$$p = \alpha(0)p_1(0) + (1 - \alpha(0))p_2(\rho/(1 - \alpha(0)) \tag{14}$$

- If $\rho > \rho_W - \rho_A$ (equivalent to $\theta < 1$), the linear and isobaric models are equivalents.
- In strong rarefaction waves, the pressure law of the liquid is modified: the gas is present, with no mass !
- Very rough model for cavitation.
- It is possible to have different sound speeds in the pure fluids.

Notes on conservative schemes

- Any standard conservative scheme is inaccurate with the linear pressure law [1].
- It does not preserve constant (u, p) states [2].
- When it does not crash, the scheme does converge ! but the precision is very bad on standard meshes [3].

---

[1] S. Karni. Multicomponent flow calculations by a consistent primitive algorithm. *Journal of Computational Physics*, 112(1):31–43, 1994.

[2] R. Abgrall. Generalisation of the Roe scheme for the computation of mixture of perfect gases. *Recherche Aérospatiale*, 6:31–43, 1988.

[3] Thierry Gallouët, Jean-Marc Hérard, and Nicolas Seguin. A hybrid scheme to compute contact discontinuities in one-dimensional Euler systems.*M2AN. Mathematical Modelling and Numerical Analysis*, 36(6):1133–1159 (2003), 2002.

Non-conservative scheme

- For the linear pressure law, we need a non-conservative approach.
- The conserved variables are $w = (\rho, \rho u)$ and the non-conservative variable is φ that satisfies

$$\varphi_t + u\varphi_x = 0. \tag{15}$$

- The conservative flux is

$$f(w, \varphi) = (\rho u, \rho u^2 + p). \tag{16}$$

A non-conservative version of the Rusanov scheme is

$$
\begin{aligned}
&\frac{w_i^{n+1}-w_i^n}{\Delta t}+\frac{f_{i+1/2}^n-f_{i-1/2}^n}{\Delta x}=0,\\
&f_{i+1/2}^n=\frac{f_i^n+f_{i+1}^n}{2}-\frac{s_{i+1/2}^n}{2}(w_{i+1}^n-w_i^n),\\
&s_{i+1/2}:\ \text{maximal wave speed at } i+1/2,\\
&\frac{\varphi_i^{n+1}-\varphi_i^n}{\Delta t}+\frac{g_{i+1/2,-}^n-g_{i-1/2,+}^n}{\Delta x}=0,\\
&g_{i+1/2,-}^n=\frac{u_i^n}{2}(\varphi_{i+1}^n-\varphi_i^n)-\frac{s_{i+1/2}^n}{2}(\varphi_{i+1}^n-\varphi_i^n),\\
&g_{i-1/2,+}^n=\frac{u_i^n}{2}(\varphi_{i-1}^n-\varphi_i^n)-\frac{s_{i-1/2}^n}{2}(\varphi_i^n-\varphi_{i-1}^n).
\end{aligned}
\tag{17}
$$

Adapted from [4] and [5].

[4] R. Saurel and R. Abgrall. A simple method for compressible multifluid flows. *SIAM Journal on Scientific Computing*, 21(3):1115–1145, 1999.

[5] F. Golay and P. Helluy. Numerical schemes for low mach wave breaking. Submitted, 2007.

- This scheme preserves constant (u, p) states and is much more accurate that a standard conservative scheme.
- A Godunov version, which is more precise, can also be written.
- Extension to second order is possible with a standard MUSCL method: the reconstructed variables may be (ρ, u, p) (in order to preserve constant (u, p) states).
- Because the last equation is non-conservative, an additional source term is needed in the second order numerical scheme.

Isobaric scheme

- A conservative approach can be employed with the isobaric pressure law (see [6], [7]) .
- The conserved variables are here $w = (\rho, \rho u, \rho\varphi)$ and the flux is $f(w) = (\rho u, \rho u^2 + p, \rho\varphi u)$.
- We can use the numerical flux of Rusanov for instance

$$f_{i+1/2}^n = \frac{f_i^n + f_{i+1}^n}{2} - \frac{s_{i+1/2}^n}{2}(w_{i+1}^n - w_i^n) \tag{18}$$

[6] Grégoire Allaire, Sébastien Clerc, and Samuel Kokh. A five-equation model for the simulation of interfaces between compressible fluids. *Journal of Computational Physics*, 181(2):577–616, 2002.

[7] G. Chanteperdrix, P. Villedieu, and Vila J.-P. A compressible model for separated two-phase flows computations. In *ASME Fluids Engineering Division Summer Meeting*. ASME, Montreal, Canada, July 2002.

- The scheme preserves constant (u, p) states.
- The second order MUSCL extension is immediate.
- The Godunov scheme is not employed (because the exact Riemann solver is too much complicated).
- But relaxation schemes based on exact Riemann solvers give more accurate results.
- The main concern is that, in some regimes, the original pressure laws are modified.

Numerical illustrations

Riemann problem with

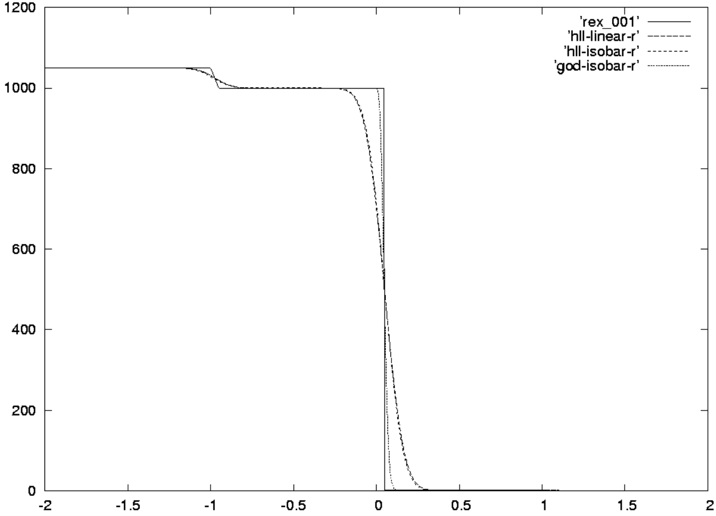
$$\begin{aligned} &\varphi_L = 0 \quad p_L = 500 \times 10^5 \text{ Pa} \quad u_L = 0 \\ &\varphi_R = 1 \quad p_R = 2118 \text{ Pa} \quad u_R = 0 \end{aligned} \tag{19}$$

500 cells, $x \in [-2, 2]$, $t = 0.001$ s.

$$\begin{aligned} p_0 &= 10^5 \text{ Pa} \\ \rho_A &= 1 \text{ kg.m}^{-3} \\ \rho_W &= 1000 \text{ kg.m}^{-3} \\ c &= 1000 \text{ m.s}^{-1} \end{aligned} \tag{20}$$

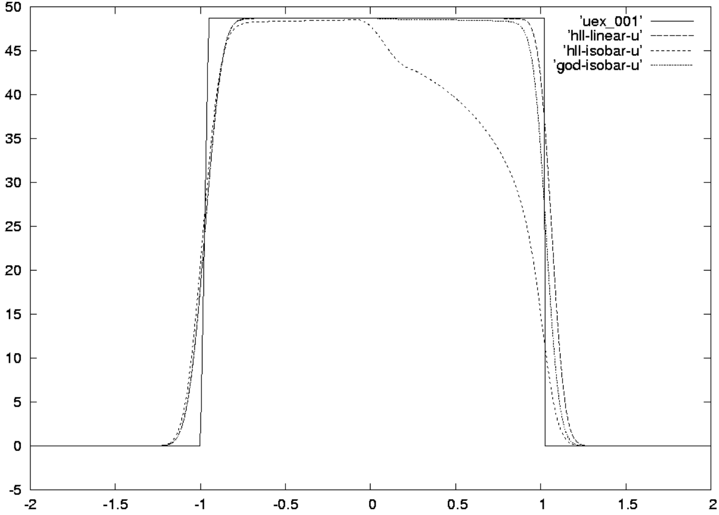
Comparison between: Rusanov with Linear or Isobaric EOS and Godunov (relaxation) with Isobaric EOS.

Density



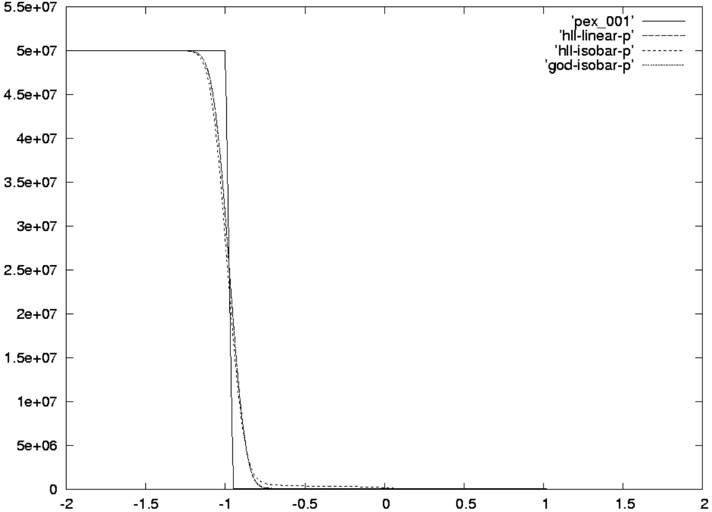
'rex_001'
'hll-linear-r'
'hll-isobar-r'
'god-isobar-r'
1200
1000
800
600
400
200
0
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2

Velocity



'uex_001'
'hll-linear-u'
'hll-isobar-u'
'god-isobar-u'
50
45
40
35
30
25
20
15
10
5
0
-5
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2

Pressure



'pex_001'
'hll-linear-p'
'hll-isobar-p'
'god-isobar-p'
5.5e+07
5e+07
4.5e+07
4e+07
3.5e+07
3e+07
2.5e+07
2e+07
1.5e+07
1e+07
5e+06
0
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2

Strong rarefaction

Riemann problem with

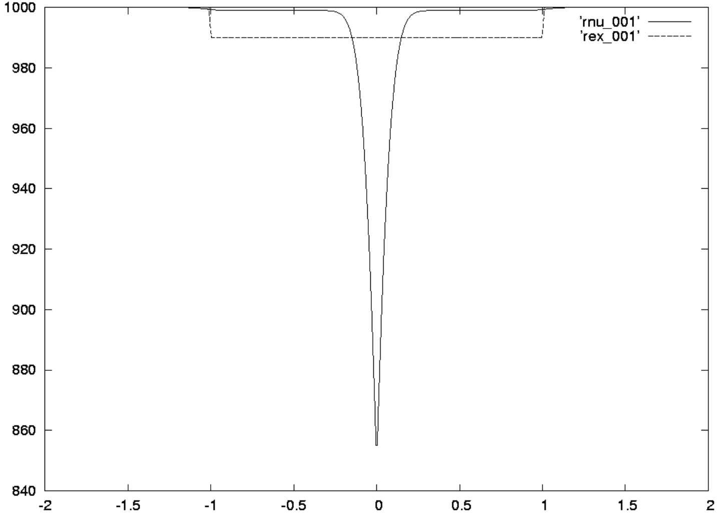
$$\begin{aligned} \varphi_L &= 0 \quad p_L = 10^5 \text{ Pa} \quad u_L = -10 \text{ m/s} \\ \varphi_R &= 0 \quad p_R = 10^5 \text{ Pa} \quad u_R = 10 \text{ m/s} \end{aligned} \tag{21}$$

500 cells, $x \in [-2, 2]$, $t = 0.001$ s.

$$\begin{aligned} p_0 &= 10^5 \text{ Pa} \\ \rho_A &= 1 \text{ kg.m}^{-3} \\ \rho_W &= 1000 \text{ kg.m}^{-3} \\ c &= 1000 \text{ m.s}^{-1} \end{aligned} \tag{22}$$

Comparison between: Exact Riemann solver with Linear pressure law and "Godunov" (relaxation) with Isobaric EOS.

Density



1000
980
960
940
920
900
880
860
840
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2
'rnu_001'
'rex_001'

A simple two-energy model

We try now to extend the previous remarks to a two-fluid model with an energy conservation law.

Conservation laws

The energy model reads

$$\begin{aligned}
&\rho_t + (\rho u)_x = 0,\\
&(\rho u)_t + (\rho u^2 + p)_x = 0,\\
&(\rho E)_t + ((\rho E + p)u)_x = 0,\\
&(\rho\varphi)_t + (\rho\varphi u)_x = 0,\\
&p = p(\rho, \rho\varepsilon, \varphi),\\
&E = \varepsilon + \frac{1}{2}u^2.
\end{aligned} \tag{23}$$

Linear pressure law

The pressure law may be

$$p = (\gamma(\varphi) - 1)\rho\varepsilon - \gamma(\varphi)\pi(\varphi), \tag{24}$$

with

$$\begin{aligned} \frac{1}{\gamma(\varphi)-1} &= \varphi\frac{1}{\gamma_A - 1} + (1-\varphi)\frac{1}{\gamma_W - 1}, \\ \frac{\gamma(\varphi)\pi(\varphi)}{\gamma(\varphi)-1} &= \varphi\frac{\gamma_A\pi_A}{\gamma_A - 1} + (1-\varphi)\frac{\gamma_W\pi_W}{\gamma_W - 1}. \end{aligned} \tag{25}$$

See [8] and [9].

---

[8] R. Saurel and R. Abgrall. A simple method for compressible multifluid flows. *SIAM Journal on Scientific Computing*, 21(3):1115–1145, 1999.

[9] F. Golay and P. Helluy. Numerical schemes for low mach wave breaking. Submitted, 2007.

General pressure law

We also have to define the energy fraction ζ and the partial specific energies ε_i by

$$\begin{aligned} &\rho\varepsilon = \alpha\rho_1\varepsilon_1 + (1-\alpha)\rho_2\varepsilon_2, \\ &\zeta = \frac{\alpha\rho_1\varepsilon_1}{\rho\varepsilon}. \end{aligned} \tag{26}$$

The pressure laws of each fluid is noted p_i. We then eliminate the volume fraction by setting

$$\begin{aligned} &p_1(\rho_1, \rho_1\varepsilon_1) = p_2(\rho_2, \rho_2\varepsilon_2), \\ &\text{or } p_1\left(\frac{\rho\varphi}{\alpha}, \frac{\zeta\rho\varepsilon}{\alpha}\right) = p_2\left(\frac{\rho(1-\varphi)}{1-\alpha}, \frac{(1-\zeta)\rho\varepsilon}{1-\alpha}\right). \end{aligned} \tag{27}$$

In this case, the evolution of the energy fraction ζ has to be provided

Koren[10] suggested to add the following equation to (23)

$$\begin{aligned} &E_i = \varepsilon_i + \frac{1}{2}u^2, \\ &(\alpha\rho_1 E_1)_t + (\alpha\rho_1 E_1 u)_x + \alpha p u_x + \varphi u p_x = 0. \end{aligned} \tag{28}$$

- This non-conservative equation gives the missing evolution of ζ.
- It is obtained from mechanical arguments (the work of the interphase drag force is computed from the common acceleration of the two fluids in the mixture region).
- It could also be deduced from a 7 equations model by Chapmann-Enskog expansions (relaxation of pressures and velocities but not of temperatures).
- The whole system is hyperbolic.

[10] E. H. van Brummelen and B. Koren. Five-Equation Model for Compressible Two-Fluid Flow. Centrum voor Wiskunde en Informatica, Report MAS-E0414, 2004.

When the two fluids are stiffened gases, it is possible to make the computations more precise. We have $p_i = p_i(\rho_i \varepsilon_i)$. It gives

$$\begin{aligned}
&\delta = \gamma_A \pi_A - \gamma_W \pi_W < 0, \\
&\gamma = \zeta \gamma_A + (1-\zeta)\gamma_W, \\
&r = (\delta + (\gamma - 1)\rho\varepsilon)^2 - 4\delta(\gamma_A - 1)\zeta\rho\varepsilon, \\
&\alpha(\zeta) = \frac{\delta + (\gamma-1)\rho\varepsilon - \sqrt{r}}{2\delta}, \\
&\alpha(1) = 1, \\
&\alpha(0) = \begin{cases} 0 & \text{if} \quad (\gamma-1)\rho\varepsilon > -\delta, \\ 1 + \frac{(\gamma-1)\rho\varepsilon}{\delta} & \text{if} \quad (\gamma-1)\rho\varepsilon < -\delta. \end{cases}
\end{aligned} \tag{29}$$

We find the same behavior as in the isothermal case (the gas can fill a positive volume with no energy).

Non-conservative scheme

The conserved variables are $w = (\rho, \rho u, \rho E)$ and the non-conservative variable is φ that satisfies

$$\varphi_t + u\varphi_x = 0. \tag{30}$$

The conservative flux is

$$f(w, \varphi) = (\rho u, \rho u^2 + p, (\rho E + p)u). \tag{31}$$

A non-conservative version of the Rusanov scheme is

$$
\begin{aligned}
&\frac{w_i^{n+1}-w_i^n}{\Delta t}+\frac{f_{i+1/2}^n-f_{i-1/2}^n}{\Delta x}=0,\\
&f_{i+1/2}^n=\frac{f_i^n+f_{i+1}^n}{2}-\frac{s_{i+1/2}^n}{2}(w_{i+1}^n-w_i^n)\\
&s:\ \text{maximal wave speed at } i+1/2\\
&\frac{\varphi_i^{n+1}-\varphi_i^n}{\Delta t}+\frac{g_{i+1/2,-}^n-g_{i-1/2,+}^n}{\Delta x}=0,\\
&g_{i+1/2,-}^n=\frac{u_i^n}{2}(\varphi_{i+1}^n-\varphi_i^n)-\frac{s_{i+1/2}^n}{2}(\varphi_{i+1}^n-\varphi_i^n),\\
&g_{i-1/2,+}^n=\frac{u_i^n}{2}(\varphi_{i-1}^n-\varphi_i^n)-\frac{s_{i-1/2}^n}{2}(\varphi_i^n-\varphi_{i-1}^n).
\end{aligned}
\tag{32}
$$

Isobaric scheme

We can also adapt the Rusanov scheme to the isobaric model. Setting

$$\begin{aligned} w &= (\rho, \rho u, \rho E, \rho\varphi, \alpha\rho_1 E_1) \\ f(w) &= (\rho u, \rho u^2 + p, (\rho E + p)u, \rho\varphi u, \alpha\rho_1 E_1 u) \\ B(w)w_x &= (0, 0, 0, 0, \alpha p u_x + \varphi u p_x) \end{aligned} \tag{33}$$

The system is written

$$w_t + f(w)_x + B(w)w_x = 0 \tag{34}$$

We write

$$\begin{aligned} & \frac{w_i^{n+1}-w_i^n}{\Delta t}+\frac{f_{i+1/2}^n-f_{i-1/2}^n}{\Delta x}+\frac{g_{i+1/2,-}^n-g_{i-1/2,+}^n}{\Delta x}=0, \\ & f_{i+1/2}^n=\frac{f_i^n+f_{i+1}^n}{2}-\frac{s_{i+1/2}^n}{2}(w_{i+1}^n-w_i^n) \\ & s: \text{ maximal wave speed at } i+1/2 \\ & g_{i+1/2,-}^n=\frac{1}{2}\left(0,0,0,0,\alpha_i^n p_i^n(u_{i+1}^n-u_i^n),\varphi_i^n u_i^n(p_{i+1}^n-p_i^n)\right), \\ & g_{i-1/2,+}^n=\frac{1}{2}\left(0,0,0,0,\alpha_i^n p_i^n(u_{i-1}^n-u_i^n),\varphi_i^n u_i^n(p_{i-1}^n-p_i^n)\right). \end{aligned} \tag{35}$$

Precision issue

Riemann problem with

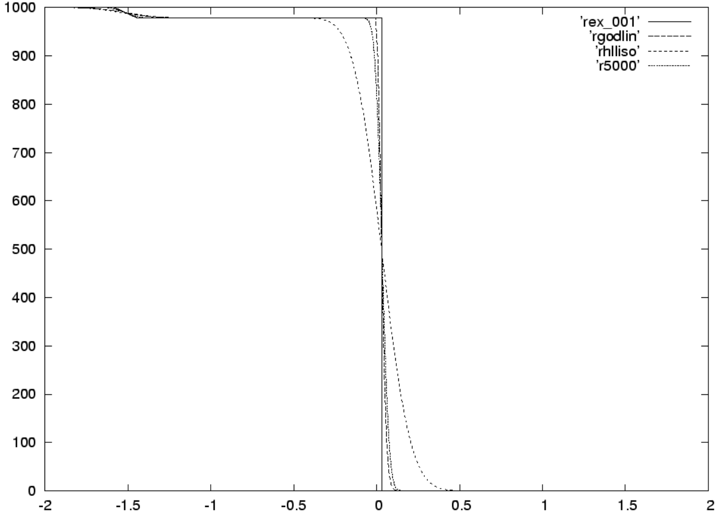
$$\begin{aligned} &\varphi_L = 0 \quad p_L = 500 \times 10^5 \text{ Pa} \quad u_L = 0 \quad \rho_L = 1000 \text{ kg/m}^3 \\ &\varphi_R = 1 \quad p_R = 2118 \text{ Pa} \quad u_R = 0 \quad \rho_R = 0.026077 \text{ kg/m}^3 \end{aligned} \tag{36}$$

500 cells (or 5000 cells), $x \in [-2, 2]$, $t = 0.001$ s.

$$\begin{aligned} \pi_A &= 0 \\ \gamma_\text{A} &= 1.4 \\ \gamma_W &= 7.15 \\ \pi_W &= 3 \times 10^8 \text{ Pa} \end{aligned} \tag{37}$$

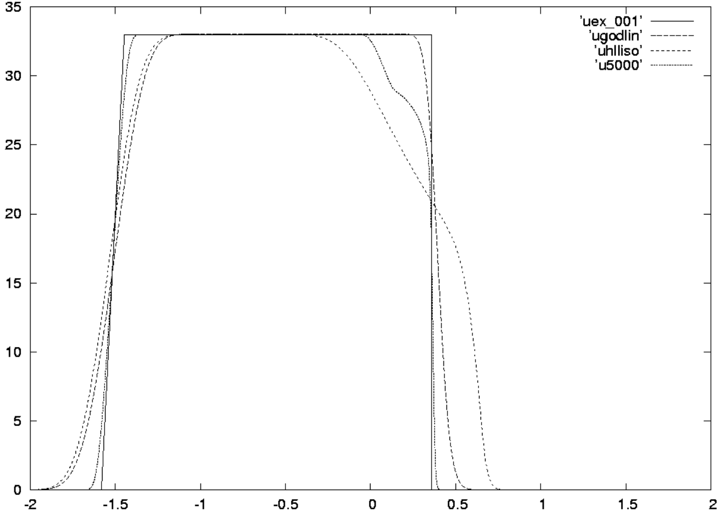
Comparison between: Rusanov with Isobaric EOS and Godunov with Linear EOS.

Density



'rex_001'
'rgodlin'
'rhlliso'
'r5000'
1000
900
800
700
600
500
400
300
200
100
0
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2

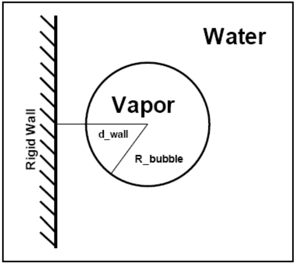
Velocity



'uex_001'
'ugodlin'
'uhlliso'
'u5000'
35
30
25
20
15
10
5
0
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2

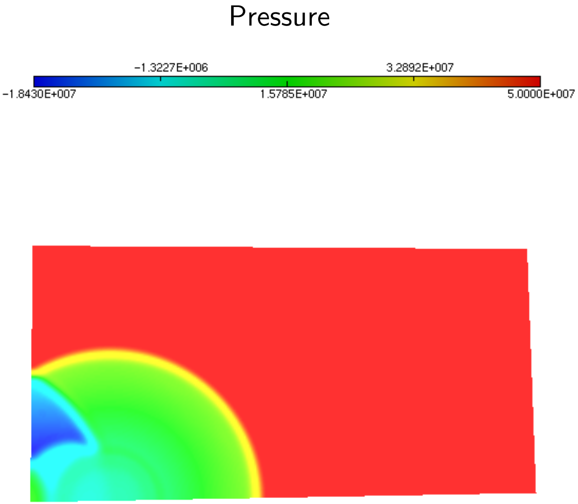
2D Numerical applications

Bubble collapse

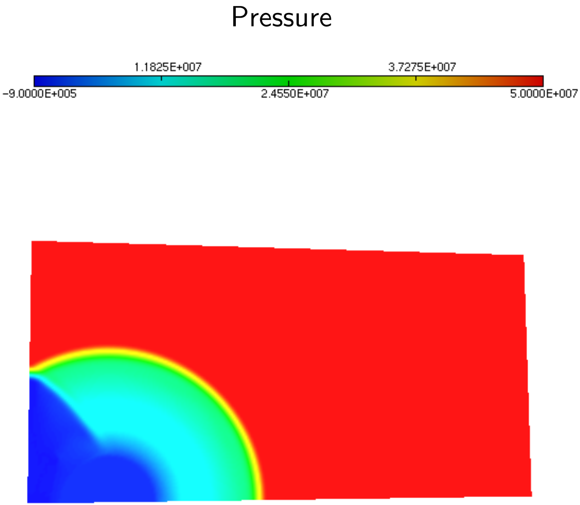


$R_{bubble} = 1$ mm
$d_{wall} = 1.5$ mm
t=1.9×10^{-6} s
Second order MUSCL "Godunov", isothermal linear or isobaric EOS

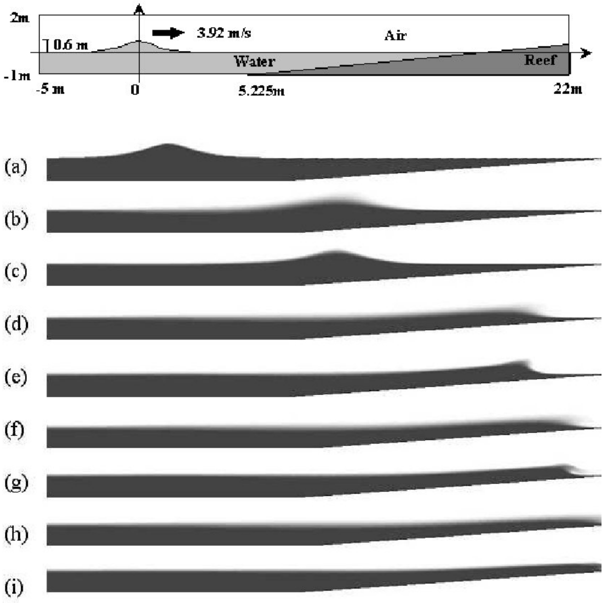
Linear isothermal pressure law



Isobaric isothermal pressure law



Wave breaking



Conclusion

- It is possible to use a conservative approach in two-fluid flows;
- It seems to imply a modification of the pressure law in strong rarefaction waves;
- The precision of the isobaric two-energy model has still to be improved (second order + relaxation + better Riemann solver);
- Multiscale grid adaptation;
- There are still open questions in the modeling: reality of negative pressures? neglecting or not the mass transfer? if not, is it instantaneous? *etc.*

Grégoire Allaire, Sébastien Clerc, and Samuel Kokh.
A five-equation model for the simulation of interfaces between compressible fluids.
Journal of Computational Physics, 181(2):577–616, 2002.

Thierry Gallouët, Jean-Marc Hérard, and Nicolas Seguin.
A hybrid scheme to compute contact discontinuities in one-dimensional Euler systems.
M2AN. Mathematical Modelling and Numerical Analysis, 36(6):1133–1159 (2003), 2002.

F. Golay and P. Helluy.
Numerical schemes for low mach wave breaking.
Submitted, 2007.

S. Karni.
Multicomponent flow calculations by a consistent primitive algorithm.
Journal of Computational Physics, 112(1):31–43, 1994.

R. Saurel and R. Abgrall.
A simple method for compressible multifluid flows.
SIAM Journal on Scientific Computing, 21(3):1115–1145, 1999.

E. H. van Brummelen and B. Koren.
Five-Equation Model for Compressible Two-Fluid Flow.
Centrum voor Wiskunde en Informatica, Report MAS-E0414, 2004.

G. Chanteperdrix, P. Villedieu, and Vila J.-P.
A compressible model for separated two-phase flows computations.
In *ASME Fluids Engineering Division Summer Meeting*. ASME, Montreal, Canada, July 2002.

R. Abgrall.
Generalisation of the Roe scheme for the computation of mixture of perfect gases.
Recherche Aérospatiale, 6:31–43, 1988.