Investigation of an implicit solver for the simulation of bubble oscillations using Basilisk

D. Fuster[1,*] and S. Popinet[1]

[1] Sorbonne Universités, UPMC Univ Paris 06, CNRS, UMR 7190
Institut Jean Le Rond d'Alembert, F-75005 Paris, France

Abstract

In this work we investigate an extension of an implicit all-Mach formulation using the Volume of Fluid (VOF) method. The numerical scheme is implemented in Basilisk [1], an open source program widely used and extensively validated for various problems involving multiple phases in the incompressible limit that allows for Adaptive Mesh Refinement using octree grids. The numerical method is adapted to ensure that the numerical scheme exactly recovers the classical fractional step method used for incompressible fluids. The new formulation is shown to capture well the dynamic response of bubbles in a liquid by validating it in two different scenarios: (a) The linear oscillation of a bubble in a slightly compressible liquid and (b) the Rayleigh collapse problem.

Keywords: CFD, Numerical methods, multiphase flows, bubble dynamics.

1 Introduction

The development of robust and accurate compressible codes for multiphase flows is important for a better understanding of processes related to wave propagation and cavitation. All-Mach formulations have been proposed by various authors (see for example [2]). The main advantage of these solvers is that it is possible to solve problems in which one of the phase (e.g. liquid) is considered as an incompressible substance circumventing the classical timestep restriction of solvers based on the solution of Riemann problem. Another advantage of these solvers is that it naturally recover the method developed to solve the Navier-Stokes equations for multiphase flows in the incompressible limit. In this work we present preliminary results on the performance of a variant of this method implemented in Basilisk, an open free-software for the solution of the fluid equations that allows for mesh adaptation. Two classical problems related to the dynamic response of bubbles in liquids are used: The linear oscillation of a bubble in a slightly compressible liquid and The Rayleigh collapse problem. The robustness of the method is shown for the collapse of a gas bubble in water induced by a shock wave.

2 Modelling equations

In this work we solve for the Navier-Stokes equations neglecting surface tension effects:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \tag{1}$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla p + \nabla \cdot \tau' \tag{2}$$

where $\tau' = \mu \left(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T\right) - \frac{2}{3}\mu \nabla \cdot \boldsymbol{u} \delta$. In the compressible framework we need to add any form of the energy equation. For instance, in absence of thermal diffusion, the total energy equation is,

$$\frac{\partial \rho e + 1/2 \rho \boldsymbol{u}^2}{\partial t} + \nabla \cdot (\rho e \boldsymbol{u} + 1/2 \rho \boldsymbol{u}^2) = -\nabla \cdot (\boldsymbol{u} p) + \nabla \cdot (\tau' \boldsymbol{u}). \tag{3}$$

*Corresponding author, Daniel Fuster: fuster@dalembert.upmc.fr

The system is closed by adding an state equation that can establishes the relation between the various thermodynamic variables. From the state equation we can determine various fluid properties such as the speed of sound $c = \left(\frac{\partial p}{\partial \rho}\right)_{S=cte}$ and the thermal dilatation coefficient $\beta_T = \frac{-1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_p$.

In the all-Mach formulation we rewritte the continuity equation to express density derivatives as a function of pressure and temperature derivatives. The density variations between two thermodynamic states can be obtained as a sum of the changes of density in an isothermal process plus the density change in an isobaric process, $d\rho = \left(\frac{\partial \rho}{\partial p}\right)_T dp + \left(\frac{\partial \rho}{\partial T}\right)_p dT$. Using the definitions of the speed of sound, the polytropic coefficient, γ and the thermal dilatation coefficient we find [3]

$$d\rho = \frac{\gamma}{c^2} dp - \rho \beta dT. \tag{4}$$

The temperature changes can be obtained from the internal energy equation, which in absence of thermal diffusion effects is written as

$$\rho c_p \frac{DT}{Dt} = \beta_T T \frac{Dp}{Dt}. \tag{5}$$

Using Eqs. 4-5 we express the density changes in the continuity equation as a function of pressure changes

$$\left[\frac{\gamma}{\rho c^2} - \frac{\beta_T^2 T}{\rho c_p}\right] \frac{Dp}{Dt} = -\nabla \cdot \boldsymbol{u}. \tag{6}$$

Note that in the limiting situation of an ideal gas, where $c = \sqrt{\gamma R T}$ and $\beta_T = 1/T$, and water $c \approx 1500$ m/s and $\beta_T \approx 0$, it is easily verified that $\frac{1}{\rho c^2} = \left[\frac{\gamma}{\rho c^2} - \frac{\beta_T^2 T}{\rho c_p}\right]$.

In the case of two phase mixtures, we need to add an advection equation for the evolution of the volume fraction for each phase,

$$\frac{\partial f}{\partial t} + \boldsymbol{u} \cdot \nabla f = 0. \tag{7}$$

3 Numerical method

In this work we are interested in investigating the time-split scheme that solves the set of equations above in two steps: The advection and the projection step.

In the *advection step* we solve for the advection of the color function f rewritting it as

$$\frac{f^{n+1} - f^n}{\Delta t} + \nabla \cdot (\boldsymbol{u} c) = c \nabla \cdot \boldsymbol{u}. \tag{8}$$

This equation is solved using the Volume of Fluid (VOF) method proposed by Weymouth & Yue [4], where we obtain the updated value of f from the flux, uf, obtained geometrically using the onto-cell implicit linear mapping of the interface. The advection step for the rest of the conservative variables is

$$\frac{\rho^{n+1} - \rho^n}{\Delta t} + \nabla \cdot (\rho u) = 0 \tag{9}$$

$$\frac{(\rho \boldsymbol{u})^* - (\rho \boldsymbol{u})^n}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} \boldsymbol{u}) = 0 \tag{10}$$

$$\frac{(\rho e + 1/2 \rho \boldsymbol{u}^2)^* - (\rho e + 1/2 \rho \boldsymbol{u}^2)^n}{\Delta t} + \nabla \cdot (\rho e \boldsymbol{u} + 1/2 \rho \boldsymbol{u}^2) = 0. \tag{11}$$

This step is solved with a Bell-Collela-Glaz advection scheme, where the flux of each conservative quantity is computed separately for each phase using the flux of f. This ensures the consistency on the advection of the various conservative quantities and the transport of the color function f avoiding any diffusion of the conservative quantities during the advection step.

The solution of the equation for pressure (Eq. 6) is also split in time, therefore, a priori one needs to solve for $\frac{Dp}{Dt} = 0$ to obtain a provisional pressure p^* in the advection step. However, this pressure is typically obtained from the provisional value of the total energy obtained after advection using the equation of state.

In the *projection step* we take the divergence of the remaining terms in the momentum equation and we replace the expression of the divergence at the end of the time-step as a function of the pressure temporal derivative given by Eq. 6. Thus, we obtain a Helmholtz-Poisson equation for pressure that is solved with the multigrid solver available in Basilisk

$$\left[\frac{\gamma}{\rho c^2} - \frac{\beta_T^2 T}{\rho c_p}\right] \frac{p^{n+1} - p^*}{\Delta t} + \nabla \cdot \boldsymbol{u}^* = \nabla \cdot \left(\frac{\Delta t}{\rho} \nabla p\right). \tag{12}$$

Once the pressure is obtained we update the value of velocity and total energy as

$$\boldsymbol{u}^{n+1} = \boldsymbol{u}^* - \frac{\Delta t}{\rho} \nabla p, \tag{13}$$

$$(\rho e + 1/2 \rho \boldsymbol{u}^2)^{n+1} = (\rho e + 1/2 \rho \boldsymbol{u}^2)^* - \nabla \cdot (\boldsymbol{u} p) \Delta t + \nabla \cdot (\tau' \boldsymbol{u}) \, \Delta t. \tag{14}$$

4 Results

4.1 Linear oscillations

We start investigating the response of a bubble to a low amplitude sinusoidal wave. We take the bubble radius R_0, the bubble natural resonance frequency $\omega_N = \frac{1}{R_0}\sqrt{\frac{3\gamma p_0}{\rho_l}}$ and the liquid's density as characteristic values of the problem. The bubble is placed at the center of a cubic domain of length $L/R_0 = 2560$. The nondimensional reference pressure is $p_0^* = 1$ and the initial gas density is $\frac{\rho_g}{\rho_l} = 10^{-3}$. We initialize a traveling planar sinuisoidal pressure wave of wavelength $\lambda^* = \lambda/R_0 = 640$ in the liquid. The amplitude of the pressure wave is initialized to a very small value to guarantee that the response of the bubble is dominated by linear terms. The nondimensional speed of sound is $c_l^* = 146.5$, which implies that $\frac{\omega}{\omega_N} = c_l^*/\lambda^* = 0.25$. The maximum resolution is applied close to the bubble interface where the grid size is $\Delta x^* = 0.156$, which gives around 12 points per diameter. The grid is coarsened far from the bubble.

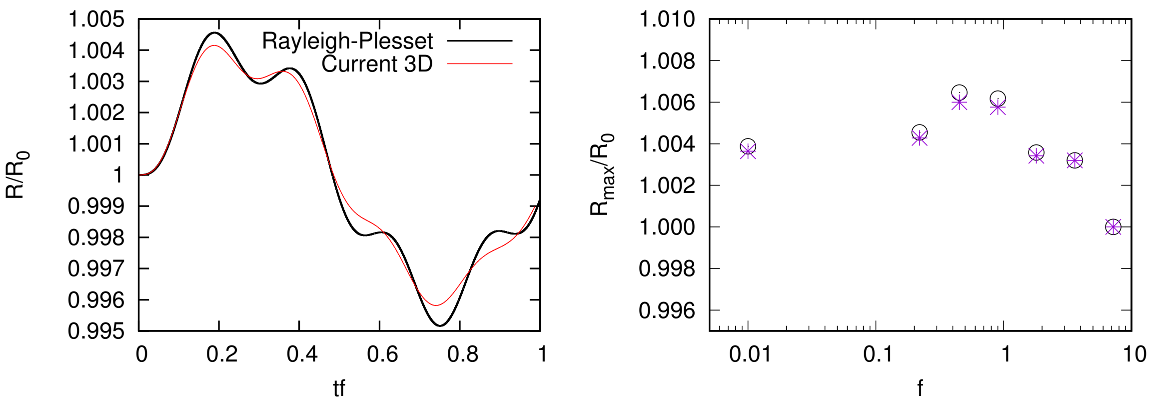
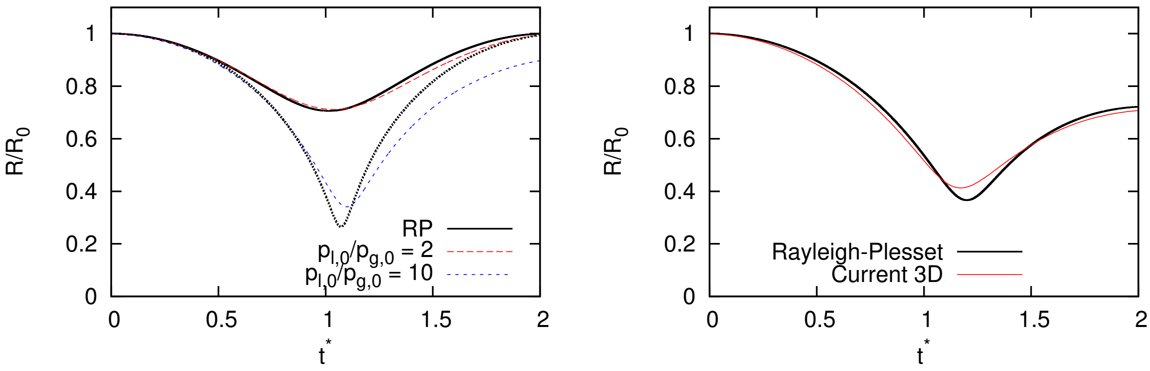


Figure 1: Left: Temporal evolution of the averaged bubble radius compared with the Rayleigh-Plesset model for the low frequency limit case $\frac{\omega}{\omega_N} = 0.25$. Right: Amplitude of the bubble oscillation as a function of the excitation frequency with the current method and the Rayleigh-Plesset model.

Figure 1 compares the evolution of the averaged radius defined as $R_{avg} = \left(\frac{V_{bubble}}{4/3\pi}\right)^{1/3}$ with the solution obtained by the Rayleigh-Plesset equation. We obtain good agreement even for the relatively low resolution used. In the same figure we also compare the maximum radius reached during the first cycle of the bubble oscillation as a function of frequency for both, the current 3D numerical simulations and the solution obtained using a Rayleigh-Plesset model. The bubble remains frozen at large frequencies, it reaches an asymptotic limit for low frequency oscillations and the amplitude of the oscillation is maximum at resonance conditions. Good agreement is found between the two models irrespective of the excitation frequency used.

4.2 Rayleigh collapse problem

The Rayleigh collapse problem is a model problem that considers the collapse of an spherical bubble at initial pressure $p_{g,0}$ in a liquid where the initial pressure is set to $p_{l,0}$. In this case we use the initial radius R_{max}, the Rayleigh collapse time $t_c = 0.915 R_{max}\sqrt{\frac{\rho_l}{\Delta p}}$ and the liquid's density as characteristic values of the problem. The initial gas density is $\rho_g^* = 10^{-3}$ in all cases and the nondimensional liquid's speed of sound is $c_l^* = 50$. A large domain, $L/R_0 = 200$ is used to avoid the influence of boundaries on the dynamic response of the bubble. Fixing these parameters, the solution of the problem depends on the ratio between the initial liquid pressure and gas pressure and the Reynolds number $\mathrm{Re} = \frac{\sqrt{\Delta p \rho_l} \mathrm{R}_{\mathrm{max}}}{\mu_l}$, defined using the characteristic velocity $U_c = 0.915 R_{max}/t_c$. In this case the minimum grid size is set to $\Delta x^* = 0.012$ (around 160 grid points per diameter).



(a) Re = ∞ (b) Re = 100

Figure 2: Bubble radius evolution for two different collapse intensities, $p_{l,0}/p_{g,0} = 2$ and $p_{l,0}/p_{g,0} = 10$. Color lines represent the solution obtained with current 3D simulations, black lines represent the solution obtained with a Rayleigh Plesset model.

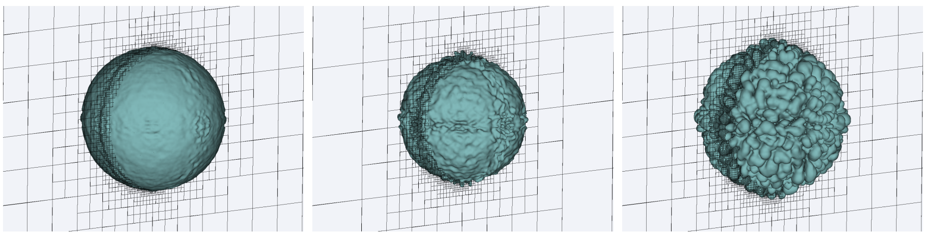


Figure 3: Evolution of the bubble interface for $p_{l,0}/p_{g,0} = 2$ and Re $= \infty$ at $t^* = \frac{2}{3}, 1, \frac{4}{3}$.

Figure 2a shows good agreement between the numerical results and the results obtained from the Rayleigh-Plesset equation for the case of a low intensity collapse ($p_{l,0}/p_{g,0} = 2$) in the inviscid case.

The three dimensional numerical simulation shows the development of a Rayleigh-Taylor instability that become especially visible right after the instant of minimum radius, when the light gas phase pushes the heavy liquid surrounding it (Fig 3). In absence of viscous and surface tension effects the bubble is always unstable during these instants. The role of the Rayleigh-Taylor instability on the bubble collapse becomes more relevant as the intensity of the collapse is increased, which may be part of the reason why the full 3D simulation and the solution obtained with a perfectly spherical bubble (Rayleigh-Plesset model) do not fit well for $p_{l,0}/p_{g,0} = 10$ after the gas start exerting resistance to the bubble collapse. The possibility to dynamically adapt the grid is critical to accurately capture the development of interfacial instabilities during the collapse process.

It is possible to suppress the development of the Rayleigh-Taylor instability by adding viscosity. Simulations at $p_{l,0}/p_{g,0} = 10$ and Re=100 reveal that the bubble collapse is almost perfectly spherically symmetric (not shown here). In this case the evolution of the bubble radius predicted by the Rayleigh-Plesset model is in agreement with the result obtained from the full 3D simulations (Figure 2b).

4.3 2D Shock wave/bubble interaction problem

Following previous works (see for example [5]), the roboustness of the solver for strong collapses is tested using the 2D interaction of a shock wave with a gas bubble in water. The strength of the incoming wave moving from left to right is set to $p_{shock}/p_0 = 1000$. The rest of variables are initialized according to the Rankine-Hugoniot conditions. Figure 4 shows the violent process of the bubble collapse. A characteristic jet previously observed in this type of simulations generate small bubbles as a consequence of the breakup of the gas sheet when the jet traverses the bubble.

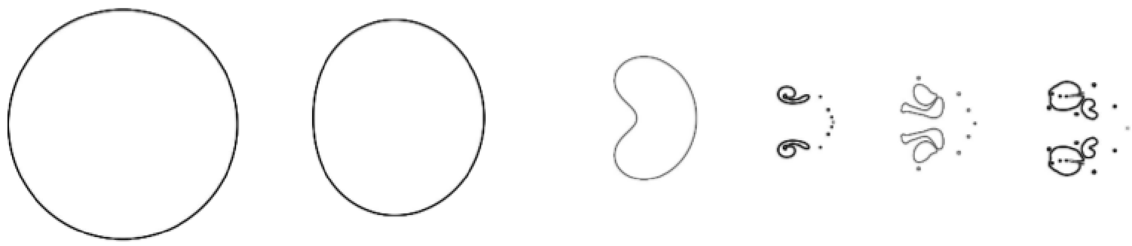


Figure 4: Interface contours for the 2D Shock wave-bubble interaction problem at different instants. $p_{shock}/p_0 = 1000$, $\rho_{g,0}/\rho_{l,0} = 10^{-3}$.

5 Conclusions

In this work we present an extension of an implicit all-Mach formulation using the Volume of Fluid (VOF) method. The discretized numerical scheme is implemented in Basilisk, an open source software widely used and extensively validated for various problems involving multiple phases in the incompressible limit that is parallel and allows for Adaptive Mesh Refinement (AMR) using octree grids. The current numerical scheme accounts for compressible effects ensuring that it exactly recovers the classical fractional step method used for incompressible fluids.

The new formulation is shown to perform well in cases involving multiple phases related to the dynamic response of bubbles in a liquid. The code is validated in two different scenarios: The linear oscillation of a bubble in a slightly compressible liquid and the Rayleigh collapse problem. Finally, the code is shown to be robust in the case of the shock induced collapse of a gas bubble in water.

References

[1] *www.basilisk.fr*

[2] S.Y. Yoon, T. Yabe *The unified simulation for incompressible and compressible flow by the predictor-corrector scheme based on the CIP method*, J. Comp. Phys, 119, 149-158, 1999.

[3] D. Fuster. *Modelling and numerical simulation of the dynamics of liquid-bubble cavitating systems with chemical reaction processes*, PhD dissertation, University of Zaragoza, 2007.

[4] G.D. Weymouth, D.K.P. Yue. *Conservative volume-of-fluid method for free-surface simulations on Cartesian-grids*, J. Comp. Phys, 229, 8, 2010.

[5] E. Johnsen, T. Colonius. *Numerical simulations of non-spherical bubble collapse*, J. Fluid Mech, 629, 231-262, 2009.