Numerical study of bubble and droplet dynamics with partitioned solvers

Joris Degroote

Supervisor(s): Jan Vierendeels, Erik Dick

Abstract— **This article explains how bubbles and droplets can be simulated using partitioned solvers. The flow in the liquid is simulated with a black box fluid solver. A structural solver calculates the interface position. As the interaction between both solvers is strong, implicit coupling with implicit stepping in the coupling iterations of a time step is required to avoid divergence. Therefore, a reduced order model of the black box fluid solver, based on modal analysis, is build up during the coupling iterations. This model is applied to an oscillating liquid droplet, a bubble rising in stagnant liquid and the formation of a bubble at the end of a vertical needle, submerged in quiescent water.**

Keywords— **CFD, modal analysis, fluid-structure interaction, bubble, droplet**

I. Introduction

THE dynamics of bubbles and droplets result from the interaction of surface tension on the interface, conceived as a zero thickness structure, and the fluid flow on both sides of the interface. The point of view of Fluid-Structure Interaction (FSI) algorithms is thus a logical choice. Using the FSI nomenclature, most techniques commonly used to simulate bubbles and droplets are monolithic schemes. The position of the interface and the fluid flow are calculated in a single code.

Here, a partitioned approach is presented. The flow in the liquid is simulated using a black box commercial code. The position of the interface is calculated with a structural solver. The solvers for axisymmetric problems without mass transfer between the gas and the liquid are defined in Section II. As the interaction between both solvers is strong, subsequent calls of the structural solver and the fluid solver, lead to divergence. Implicit stepping in the coupling iterations requires the Jacobian of the fluid solver. The Jacobian of the black box fluid solver is not available. Thus, a reduced order model, based on modal analysis, is build up during the coupling iterations of a time step in order to have an approximation for the Jacobian. This coupling procedure, developed by Vierendeels [1], is explained in Section III. Some results are presented in Section IV.

II. Solvers

A. Structural solver

If viscous stresses on the interface and the variation of the surface tension coefficient σ are neglected, equation (1) must be satisfied on the interface.

$$P + \sigma\kappa = 0 \tag{1}$$

with P the pressure jump across the interface and κ the surface curvature, which is calculated from the principal radii of curvature, R_1 and R_2.

Department of flow, heat and combustion mechanics, Ghent University (UGent), Gent, Belgium. E-mail: Joris.Degroote@UGent.be .

The interface of an axisymmetric bubble or droplet is represented with a curve in a meridional plane, discretised with N nodes. The coordinates of the nodes are placed in a vector $\boldsymbol{X}$, the pressure jump P in the nodes make up the vector $\boldsymbol{P}$. The left hand side of equation (1), evaluated in node i is further indicated as $g_{1,i}(\boldsymbol{X}, \boldsymbol{P})$. A second equation $g_{2,i}(\boldsymbol{X}) = 0$ in node i keeps the nodes equidistant. The expressions g_1 and g_2 for all nodes on the interface are written as a vector:

$$\mathbf{G}(\boldsymbol{X}, \boldsymbol{P}) = 0 \tag{2}$$

The code to solve equation (2) for $\boldsymbol{X}$ is called the *structural solver*.

B. Fluid solver

The pressure in the gas is modelled uniform in space. When the gas is the surrounding fluid, the pressure is constant. For a bubble, the gas pressure is calculated from the mass, volume ($\boldsymbol{X}$) and temperature using the ideal gas law.

To calculate the pressure distribution on the liquid side of the interface, `Fluent 6.1` is used. However, the motion of the boundary representing the bubble or droplet is not known in advance. The solver must be capable to compute the pressure distribution on the liquid side of the interface, given a deformation of this interface.

The call of `Fluent`, followed by the conversion of the pressure distribution on the liquid side of the interface into $\boldsymbol{P}$, is called the *fluid solver*, represented by equation (3).

$$\boldsymbol{P} = \mathbf{F}(\boldsymbol{X}) \tag{3}$$

III. Coupling procedure

The calculations start from time step n so $\boldsymbol{X}^n$, $\boldsymbol{P}^n$ and $\boldsymbol{V}^n$ are known, with $\boldsymbol{V}$ denoting the vector with the node velocities. Next, a subscript k is used to indicate the coupling iteration in a time step. Now is explained how $\boldsymbol{X}^{n+1}$ and $\boldsymbol{P}^{n+1}$ are obtained:

- **First coupling iteration** ($k = 1$)

A first guess for the position of the interface in time-step $n + 1$, denoted $\boldsymbol{X}_1^{n+1}$, is calculated using an explicit forward Euler scheme:

$$\boldsymbol{X}_1^{n+1} = \boldsymbol{X}^n + \boldsymbol{V}^n \Delta t \tag{4}$$

with Δt the time step. $\boldsymbol{P}_1^{n+1}$ is obtained from the fluid solver:

$$\boldsymbol{P}_1^{n+1} = \mathbf{F}^{n+1}\left(\boldsymbol{X}_1^{n+1}\right) \tag{5}$$

- **Second coupling iteration** ($k = 2$)

To simplify notation, the superscript $n + 1$ is dropped. With $\boldsymbol{P} = \boldsymbol{P}_1$, Newton's method is used to solve equation (2) for $\tilde{\boldsymbol{X}}_2$.

$\boldsymbol{X}_2$ is then obtained as $\boldsymbol{X}_1 + \omega\left(\tilde{\boldsymbol{X}}_2 - \boldsymbol{X}_1\right)$, with $\omega = 0.05$. $\boldsymbol{P}_2$ is calculated with the fluid solver.

$$\boldsymbol{P}_2 = \mathbf{F}\left(\boldsymbol{X}_2\right) \tag{6}$$

• **Coupling iteration** $k+1$ ($k \geq 2$)
At this point, k positions of the interface with the corresponding pressure distributions are known. They can be converted in $k-1$ displacement mode(s) $\boldsymbol{v}_m = \boldsymbol{X}_m - \boldsymbol{X}_k$, with m running from 1 to $k-1$, and the associated mode(s) $\boldsymbol{w}_m = \boldsymbol{P}_m - \boldsymbol{P}_k$ describing the corresponding change in pressure jump. Any displacement $\Delta\boldsymbol{X}_{k+1} = \boldsymbol{X}_{k+1} - \boldsymbol{X}_k$ can be projected on the set of displacement modes, with a remainder term $\Delta\boldsymbol{X}_{remainder}$.

$$\Delta\boldsymbol{X}_{k+1} = \sum_{m=1}^{k-1} \alpha_m \boldsymbol{v}_m + \Delta\boldsymbol{X}_{remainder} \tag{7}$$

The coefficients α_m are determined with the least-squares technique, so that the remainder term is minimized.

$$\begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_{k-1} \end{bmatrix} = \begin{bmatrix} \boldsymbol{v}_1^{\mathrm{T}}\boldsymbol{v}_1 & \dots & \boldsymbol{v}_1^{\mathrm{T}}\boldsymbol{v}_{k-1} \\ \vdots & \ddots & \vdots \\ \boldsymbol{v}_{k-1}^{\mathrm{T}}\boldsymbol{v}_1 & \dots & \boldsymbol{v}_{k-1}^{\mathrm{T}}\boldsymbol{v}_{k-1} \end{bmatrix}^{-1} \begin{bmatrix} \boldsymbol{v}_1^{\mathrm{T}} \\ \vdots \\ \boldsymbol{v}_{k-1}^{\mathrm{T}} \end{bmatrix} \Delta\boldsymbol{X}_{k+1} \tag{8}$$

The distribution of the pressure jump corresponding to the position $\boldsymbol{X}_{k+1}$ can be estimated from:

$$\hat{\boldsymbol{P}}_{k+1} = \boldsymbol{P}_k + \sum_{m=1}^{k-1} \alpha_m \boldsymbol{w}_m = \hat{\mathbf{F}}(\boldsymbol{X}_{k+1}) \tag{9}$$

In this way, a reduced order model $\hat{\mathbf{F}}$ for the fluid solver is obtained. To distinguish between $\boldsymbol{P}$ coming from the reduced order model and from the actual fluid solver, a hat is used. The Jacobian of this reduced order model is given by $\begin{bmatrix} \boldsymbol{w}_1 & \dots & \boldsymbol{w}_{k-1} \end{bmatrix}$ multiplied by the right hand side of equation (8), without $\Delta\boldsymbol{X}_{k+1}$. Using the reduced order model and its Jacobian, we can solve equation (2) implicitly using Newton's method:

$$\boldsymbol{X}_{k+1,s+1} = \boldsymbol{X}_{k+1,s} - \left(\frac{\partial \mathbf{G}}{\partial \boldsymbol{X}} + \frac{\partial \mathbf{G}}{\partial \boldsymbol{P}}\frac{\partial \hat{\boldsymbol{P}}}{\partial \boldsymbol{X}}\right)^{-1} \mathbf{G}_{k+1,s} \tag{10}$$

with $\mathbf{G}_{k+1,s} = \mathbf{G}\left(\boldsymbol{X}_{k+1,s}, \hat{\boldsymbol{P}}_{k+1,s}\right)$.
Starting from the second time step, modes of the previous time step are used to get a better reduced order model. This greatly accelerates convergence.

IV. Results

A. Oscillating droplet

The small amplitude oscillation of an axisymmetric and left-right symmetric water droplet in air has been simulated. The value found for the angular frequency of the small amplitude oscillation of a water droplet with equilibrium radius $R_0 = 1.48\,\mathrm{mm}$ is $\omega = 417.49\,\mathrm{rad/s}$, which differs only 0.2 % from the linear approximation by Lamb [2].

Large amplitude oscillation has also been studied. Grid independence of the result has been proved.

B. Rising bubble

Bubble A in Table I from Hnat et al. [3], an air bubble rising in mineral oil due to gravity, has been simulated in a moving reference frame. The steady-state bubble shape is shown in Figure 1. The terminal rise velocity of 0.2390 m/s differs 11 % from the experimental value.

Fig. 1. Comparison of the experimental (left) and numerical (right) steady-state shape of bubble A in Table I from Hnat et al. [3].

C. Bubble detachment from a needle

The growth and detachment of an air bubble at the end of a vertical needle, submerged in quiescent water has also been studied. For the gas flow through the needle, a model from Oğuz et al. [4] has been used. A specific case studied experimentally by Longuet-Higgins et al. [5], has been simulated. The experimental and numerical results are compared in Figure 2.

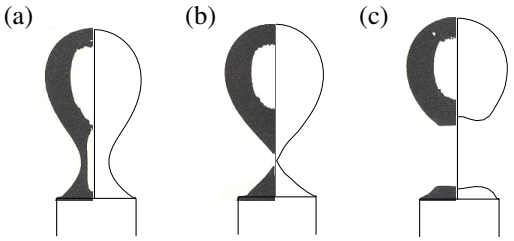

Fig. 2. Comparison of the experimental (left) and numerical (right) bubble shape at (a) -2 ms, (b) at detachment and (c) 2 ms afterwards, for a case studied experimentally by Longuet et al. [5].

V. Conclusions

The ALE description allows a very accurate representation of the interface of bubbles and droplets. The position of the interface is calculated with a structural solver using a reduced order model for the black box fluid solver. The reduced order model allows efficient implicit coupling of the partitioned solvers. The model has succesfully been applied to an axisymmetric water droplet oscillating in air and an air bubble growing and detaching from a vertical needle, submerged in quiescent water. For an air bubble rising in stagnant mineral oil, less agreement with experiments is obtained.

References

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