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4pPA7. Modeling time delay in clusters of interacting bubbles

Derek Thomas*, Yurii A. Ilinskii, Evgenia Zabolotskaya and Mark Hamilton

***Corresponding author's address: Applied Research Laboratories, The University of Texas at Austin, Austin, Texas 78758, derekcthomas@gmail.com**

Modeling the dynamics of large clusters of interacting bubbles requires that the effects of fluid compressibility be taken into account. Compressibility manifests itself through radiation damping and bubble‐bubble interactions due to time delays associated with the finite sound speed. The time delays convert the dynamical equations for interacting bubbles in an incompressible fluid from a system of nonlinear ordinary differential equations to one of delay differential equations (DDEs). Special care must be taken when integrating DDEs numerically to maintain acceptable bounds on errors. The dynamical equations determined to be most suitable for solving as DDEs were obtained using Hamiltonian mechanics [Ilinskii et al., J. Acoust. Soc. Am. 121, 786 (2007)]. These first‐order differential equations were augmented to include time delays in the bubble interaction terms and then solved numerically using a sixth‐order Runge-Kutta method with a continuous interpolant (DDE_SOLVER). The same equations were also solved without the time delays but with correction terms that account for mutual radiation damping. Comparison of the results reveals the importance of time delay in bubble‐bubble interactions as a function of the size and density of a bubble cluster.

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Introduction

Bubbles have significant effects in shock-wave lithotripsy, high intensity focused ultrasound, and histotripsy. In order to better understand the impact that bubbles have on these treatments we need a model that includes bubble interactions, includes bubble nonlinearity, is robust at high pressures and very large radial oscillations, and scales to large, distributed clusters. The ultimate goal is to simulate clusters of more than 1000 bubbles.

Methods

The model employed here is based on the model for interacting bubbles developed by Ilinskii *et al.*[1] We assume that the bubbles remain spherical and the bubbles are modeled as coupled nonlinear oscillators. Although it is possible to allow for bubble translation, translation is not explicitly considered here. Initially it is assumed that the surrounding fluid is incompressible. With these assumptions it is possible to obtain equations of motion by a Hamiltonian formalism.

After the equations of motion have been obtained, the effects of liquid compressibility are included in an *ad hoc* fashion. In an incompressible liquid, bubble interactions are instantaneous. There are two effects that must be included, radiation damping (energy lost to acoustic radiation) and time delay in bubble interactions due to acoustic propagation. The equations of motion for bubbles without time delay in bubble interaction (radiation damping is included) to first order in R/D are

$$\dot{R}_i = \frac{1}{4\pi\rho_0}\left[\frac{G_i}{R_i^3} - \sum_{j\neq i}\frac{G_j}{R_i R_j D_{ij}}\right], \tag{1a}$$

$$\begin{aligned}\dot{G}_i = \frac{1}{4\pi\rho_0}&\left[\frac{3}{2}\frac{G_i^2}{R_i^4} - \sum_{j\neq i}\frac{G_i G_j}{R_i^2 R_j D_{ij}}\right] \\ &+ 4\pi R_i^2\left(P_i - P_0 - p_{ei} - \frac{\rho_0}{4\pi c_0}\dddot{V}_i\right),\end{aligned} \tag{1b}$$

where R_i is the bubble radius, G_i is the radial momentum, and $V_i = 4\pi R_i^3/3$ is the volume of the ith bubble (the Hamiltonian coordinate system is illustrated in Fig. 1). Translation terms have been omitted for brevity. The pressure just outside the bubble wall is given by

$$P_i = \left(P_0 + \frac{2\sigma}{R_{0i}}\right)\left(\frac{R_{0i}}{R_i}\right)^{3\gamma} - \frac{2\sigma}{R_i}, \tag{2}$$

where σ is the surface tension and R_{0i} is the equilibrium bubble radius of the ith bubble in the presence of surface tension.

Energy loss from the bubble system due to acoustic radiation produced by the motion of the bubble wall is called radiation damping. In order to study the motion of bubbles in a compressibile medium, this effect must be incorporated into the model of bubble dynamics. Radiation damping is included with the $\dddot{V}_i$ term[2] where

$$\dddot{V}_i = \frac{G_i}{4\pi\rho_0^3 R_i^3}\left[R_i\frac{\partial P_i}{\partial R_i} + 2\left(P_i - P_0 - p_{ei}\right)\right] - \frac{\partial p_{ei}}{\partial t}\frac{R_i}{\rho_0} - \frac{3G_i^3}{16\pi^2\rho_0^3 R_i^9}. \tag{3}$$

When radiation damping is included in this manner, the expansion of $\dddot{V}_i$ given in Eq. (3) is necessary to maintain system stability in numerical integration.

This model neglects all interactions of $O(R^2/D^2)$ and $O(R/D)\times O(1/c_0)$. Interactions are considered to $O(R/D)$ and corrections for compressibility do not include bubble interactions.

When time delays in interactions are included in the model the system of ODEs becomes a system of delay differential equations (DDEs):

$$\dot{R}_i = \frac{1}{4\pi\rho_0}\left[\frac{G_i}{R_i^3} - \sum_{j\neq i}\frac{1}{R_i D_{ij}}\left[\frac{G_j}{R_j}\right]_{t=t-D_{ij}/c_0}\right], \tag{4a}$$

$$\begin{aligned}\dot{G}_i = {} & \frac{1}{4\pi\rho_0}\left[\frac{3}{2}\frac{G_i^2}{R_i^4} - \sum_{j\neq i}\frac{G_i}{R_i^2 D_{ij}}\left[\frac{G_j}{R_j}\right]_{t=t-D_{ij}/c_0}\right] \\ & + 4\pi R_i^2\left(P_i - P_0 - p_{ei} - \frac{\rho_0}{4\pi c_0}\dddot{V}_i\right).\end{aligned} \tag{4b}$$

DDEs require special care in numerical solution. An accurate solution is required for entire history. Additionally, the inclusion of delays can cause instability. The model equations are integrated with DDE_SOLVER.[3] This solver uses a sixth-order Runge-Kutta method with continuous interpolant. It allows for event finding (permitting bubble collisions to be modeled). The results from direct numerical integration of the model DDEs provide "ground truth" for analyzing approximations for time delay effects.

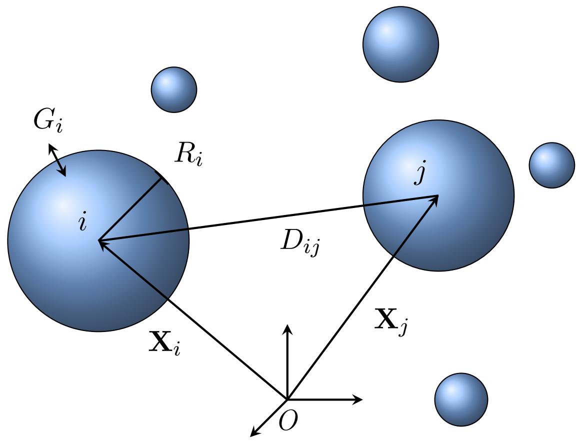

Figure 1: Coordinate system and generalized coordinates for Hamiltonian bubble model. R is the bubble radius, G is the radial momentum, the position vector of the bubble is $\mathbf{X}$. Subscripts are used to distinguish between bubbles, and D_{ij} is the separation distance between bubbles i and j.

We compare the response predicted by the equations with time delays to the response predicted without time delays for a system containing 9 bubbles randomly placed in a sphere of radius R_c. The equilibrium radius of the bubbles is $R_0 = 1\mu$m, the radius of the enclosing sphere is $R_c = 0.5$ mm. The geometry is shown in Fig. 2. The system is excited by the pulse shown on the left side of Fig. 3. The response predicted by the model with delayed interactions is compared to the response predicted by the model without delayed interactions by comparing the effective radius of the system

$$R_{eff} = \left[\sum_i R_i^3\right]^{1/3}.$$

The results are shown on the right side of Fig. 3. It can be seen that the delayed interactions significantly affect the predicted response.

Although it is possible to integrate the delay differential equations of motion numerically, the numerical solvers for delay differential equations have large memory requirements and do not scale or parallelize well. Therefore, an approximate form of the delay differential equations of motion is sought to increase the number of bubbles that can be simulated.

The model with delayed bubble interactions is approximated by adding

$$-\sum_{j\neq i} \frac{\rho_0}{4\pi c_0}\dddot{V}_j \tag{5}$$

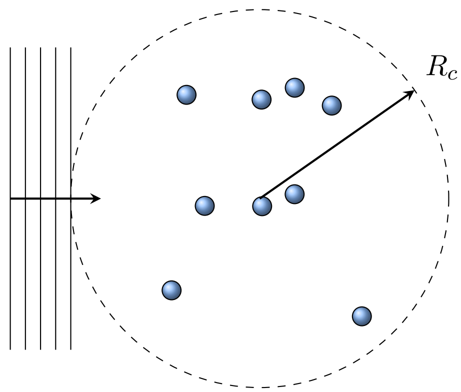

Figure 2: Bubble system geometry used to compare predicted response with and without time delays in bubble interactions.

to the pressures inside the parentheses in Eq. (1b) to obtain

$$\dot{G}_i = \frac{1}{4\pi\rho_0}\left[\frac{3}{2}\frac{G_i^2}{R_i^4} - \sum_{j\neq i}\frac{G_iG_j}{R_i^2R_jD_{ij}}\right. \\ \left. + 4\pi R_i^2\left(P_i - P_0 - p_{ei} - \sum_j \frac{\rho_0}{4\pi c_0}\dddot{V}_j\right)\right]. \tag{6}$$

Note that the sum in this expression is now over all the bubbles in the system. The third-order time derivative of the bubble volume $\dddot{V}_i$ is given by Eq. (3). A modification of this form was used by Ilinskii and Zabolotskaya.[2]

This modification is motivated by considering the pressure produced by a bubble:

$$p(r,t) = \left[\frac{\ddot{V}}{4\pi\rho_0 r}\right]_{t=t-r/c_0}. \tag{7}$$

In the neighborhood of the bubble, the pressure may be expanded in a Taylor series about $r/c_0 = 0$:

$$p(r,t) = \frac{\ddot{V}}{4\pi\rho_0 r} - \frac{\dddot{V}}{4\pi\rho_0 c_0} + O(1/c_0^2) \tag{8}$$

The interaction between the bubbles is mediated by the pressure. In the Hamiltonian formulation employed here, the interaction terms in Eqs. (1a)

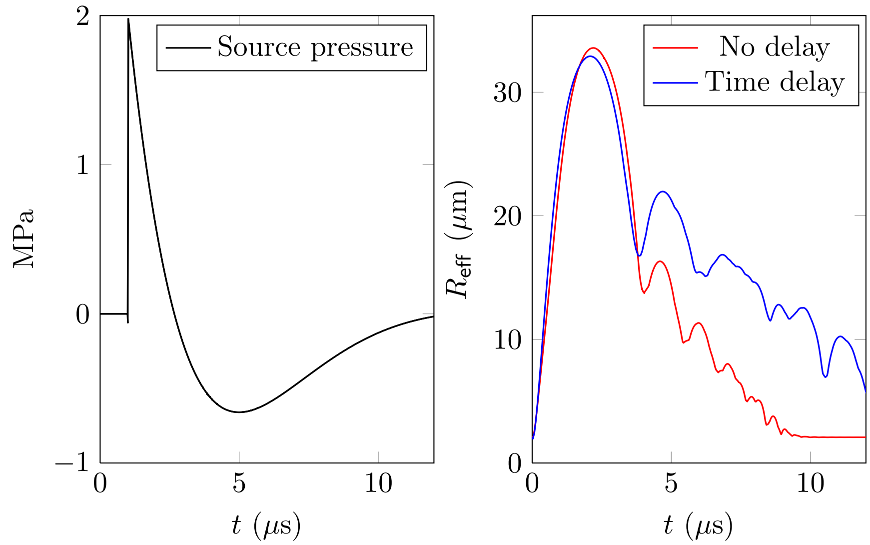

Figure 3: Input pressure waveform (left) and effective radius of the predicted system response (right) with time delays (blue) and without time delays (red) in bubble interactions.

and (1b) are equivalent to the first term in Eq. (8). The second term in Eq. (8) is the compressibility correction proposed in the previous paragraph. The compressibility correction does not depend on distance. Therefore the correction is only valid for compact clusters ($kR_c \ll 1$). It is assumed here that terms of $O(R/D) \times O(1/c_0)$ are negligible.

Results

The free and forced response predicted by the approximate form of the delay differential equations of motion (Eqs. (1a) and (6)) is compared to the response predicted by the equations of motion with delay (Eqs. (4)) and the equations of motion without delay (Eqs. (1)).

Free response

Simulations of the free response are conducted for systems of 10 bubbles placed randomly within a sphere of radius R_c The simulations are carried out for a range of values of the cluster radius R_c. The equilibrium radius of the bubbles is $R_0 = 1\mu$m. The bubbles are released together from an initial

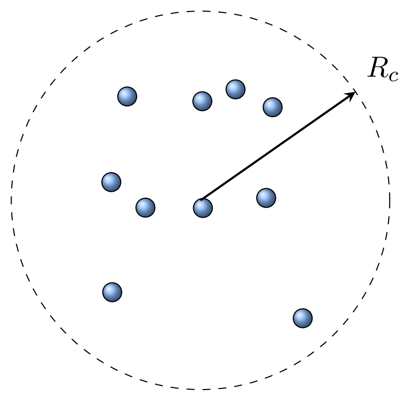

Figure 4: System geometry of 10 bubbles with equilibrium radius $R_0 = 1\mu$m used for free response simulations.

amplitude of $2R_0$. The system geometry used is shown in Fig. 4.

The effective radius for the ten bubble system in free response is shown in Fig. 5 for three different cluster sizes, $R_{\text{eff}} = 50\ \mu\text{m}, 75\ \mu\text{m}, 100\ \mu\text{m}$ (top, middle, and bottom, respectively). The predictions of three different bubble models are compared: without delays (red), with approximate delays (green), and with delays. It can be seen that for the smallest system, the agreement between the model with the approximate delays and the model with explicit delays is very good. The model without delays differs from the other two models. As the cluster size increases the spacing between the bubbles in the cluster increases and the approximations made in the model with approximate delays become less appropriate and the approximate delay equations become less accurate.

Forced response

The predictions of the three models (with delays, with approximate delays, and without delays) are compared for a larger system driven by an external acoustic source. The system consists of 30 bubbles with equilibrium radius $R_0 = 1\mu$m randomly placed in a sphere with radius $R_c = 50\mu$m. The bubbles are driven by a 10 cycle tone burst at 788 kHz with an amplitude of 1 MPa. The geometry is shown in Fig. 6. The external pressure signal is shown in the top of Fig. 7. It should be noted that the multiple scattering effects of the bubbles are already incorporated into the equations of motion.

The bottom of Fig. 7 shows the effective radius predicted without delays (red), with the approximate delay corrections (green), and with delays (blue).

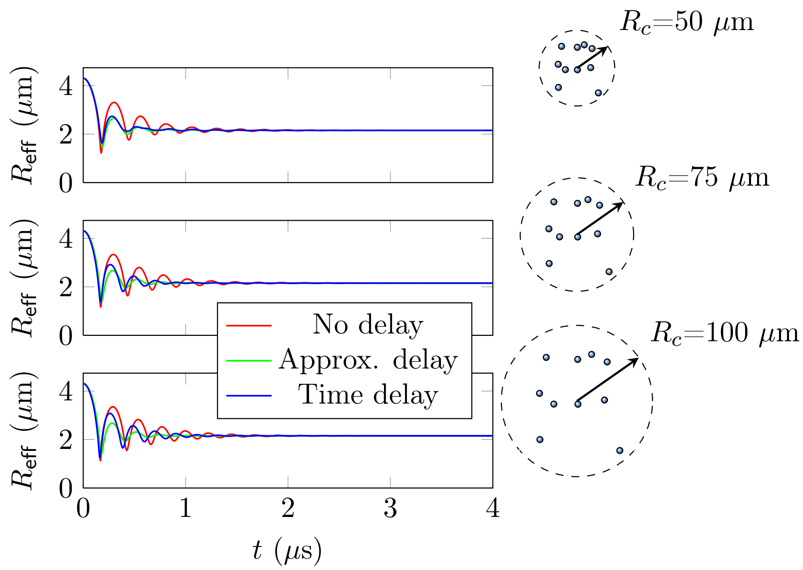

Figure 5: Effective radius predicted by model equations for free-response, in-phase motion of 10 bubbles.

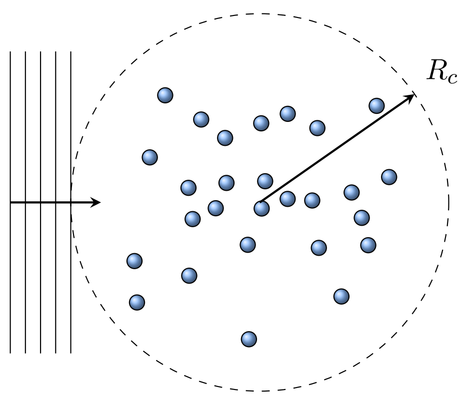

Figure 6: System of 30 bubbles used to compare the forced response predicted by the various models. The equilibrium radius of 1 μm and the cluster radius is $50R_0$.

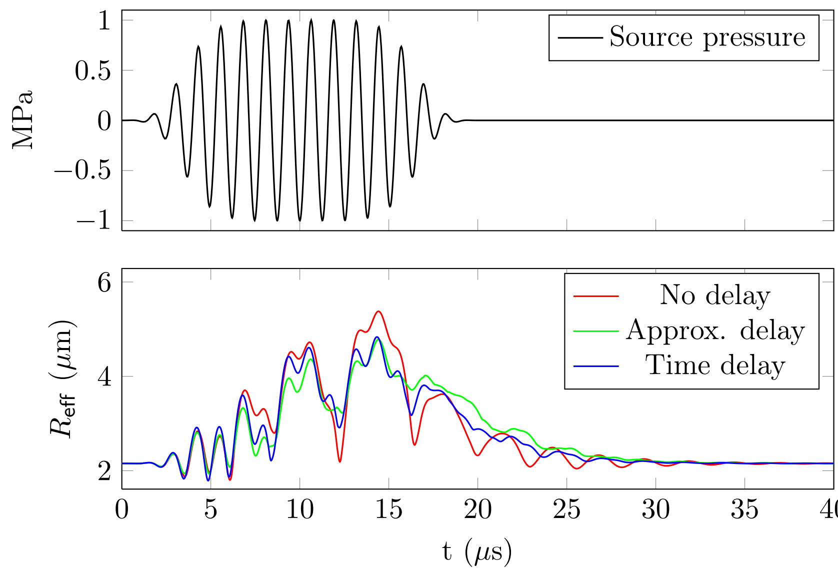

Figure 7: External source pressure (top) and effective radius of the response of the 30 bubble system shown in Fig. 6 as predicted by the model (bottom) without delays (red), with approximate delays (green), and with delays (blue).

It can be seen in the figure that the equations with the approximation to the equations with time delay (green) provide significantly better agreement with the equations with time delay (blue) than the equations without delay (red). This suggests that when modeling bubbles in a compressible medium the model without delays (Eqs. (1)) is not an appropriate choice. Either the model with delays (Eqs. (4)) or the approximate form given by Eqs. (1a) and (6) must be used.

Conclusion

It has been shown that the effects of time delay due to fluid compressibility can be significant even in compact clusters. However, the explicit inclusion of time delay in the equations of motion limits the size of clusters that can be simulated. In order to increase the number of bubbles that can be simulated while retaining the effects of liquid compressibility, an approximate form of the equations of motion with time delay was developed and compared to the equations with delays and without. The local approximation for liq-

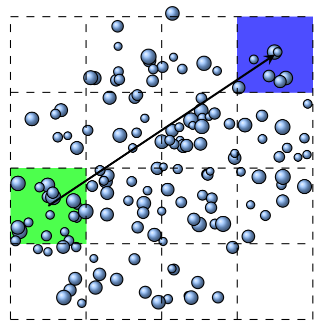

Figure 8: Illustration of proposed subclustering algorithm. Bubbles within subclusters are modeled using the approximation presented here. Delayed average pressures are used to include the effects of one subcluster on a bubble in another subcluster.

uid compressibility provides improved agreement with the predictions of the equations with delays when compared to the predictions of the equations without delay.

Future work

Future work will require an extension of the approximation for time delays presented here to account for translation.

The approximation presented here will be incorporated into a subcluster model for large bubble clusters. A large cluster will be divided into subclusters. The approximate form tested here will be used to model bubbles within the subclusters. The interaction between bubbles in different subclusters is included by computing average pressures for each subcluster and delaying the result. Thus the effect of bubbles in other subclusters acts like an external pressure source for bubbles in a subcluster. The subclustering concept is illustrated in Fig. 8.

The subclustering algorithm will significantly increase the number of bubbles that can be simulated. For explicit coupling, computation time scales as $O(N^3)$ where N is the total number of bubbles in a system. For the subcluster approach, computation time scales as $O(N_b^3 N_c^2)$ where N_b is the number of bubbles per subcluster and N_c is the number of subclusters. Thus the subclustering approach should significantly increase the attainable simulation size.

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