Optimal Ultrasonic Bubble Management in Microgravity - Draft

by

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Chapter 1

Introduction

In this paper we attempt to find the optimal forcing to translate a bubble in fluid. Specifically, we consider managing the motion of microbubbles in a negligible gravitational field. With the effective absence of gravity, there is no buoyancy and no preferential bubble motion to exploit. Bubble manipulation cannot be done passively (for example, through clever chamber design), and must then be done actively. Ultrasonic transducers are commonly used to this end, and we consider an ideal broadband transducer for this paper. We find this optimal motion by considering appropriate governing equations for the coupled radial and translational dynamics of a bubble and applying these equations as differential constraints under the calculus of variations. The process also serves as an example of how to use the calculus of variations to solve almost any dynamics problem where governing differential equations exist. The first section of this paper will address the selection of governing equations and associated assumptions, the second section the calculus of variations, the third section the pursuit of numerical solutions, and the fourth section interpretation of these solutions.

1.1 Governing Equations and Assumptions

1.1.1 Rayleigh-Plesset Equation

The radial dynamics of a bubble are governed by the well known and widely used Rayleigh-Plesset equation (RPE). We will use the RPE of Leighton [3].

$$R(t)\ddot{R}(t) + \frac{3}{2}\dot{R}^2(t) = \frac{1}{\rho}\left[P_l(t) - P_\infty(t) + \frac{R(t)}{c_l}\frac{d}{dt}(P_l - P_\infty)\right] \tag{1.1}$$

The RPE is applicable to the case of a strongly collapsing microbubble, and accounts for liquid compressibility in the damping associated with outgoing acoustic waves. In this equation $R(t)$ at its derivatives correspond the bubble radius. One particular variable of note is $P_\infty(t)$, the far-field fluid pressure. As aspiring bubble manipulators, this is our handle on the bubble and the principal term we seek to derive - everything else is only along for the ride.

Doinikov [2] proposes that the right hand side of the RPE should also include a $\frac{U^2(t)}{4}$ term - for weaker forcing $U(t)$, the far-field fluid velocity, should be small, and $U(t)^2$ be negligible. Additionally, the final term of Equation 1.2 expresses the energy lost through acoustic emission, and should also be negligible for mildly to moderately driven bubbles. The calculus of variations will produce the terms necessary to evaluate the validity of both of these assumptions. These assumptions leave us with

$$R(t)\ddot{R}(t) + \frac{3}{2}\dot{R}^2(t) = \frac{1}{\rho}\left[P_l(t) - P_\infty(t)\right]. \tag{1.2}$$

P_l in Equation 1.2 is the pressure in the liquid at the bubble wall, expressed by

$$P_l(t) = P_g(t) - \frac{4\mu\dot{R}(t)}{R(t)} - \frac{2\sigma}{R(t)} \tag{1.3}$$

where the gas pressure within the bubble is expressed by $P_g(t) = P_{go} * (R_o/R(t))^{3\kappa}$. The formulation energy tapped in dynamic gas behavior within the bubble. Additionally, we reformulate P_∞ as $P_o(1 - F(x/c_l - t))$, where $F(x/c_l - t)$ is a dimensionless overpressure in the form of a traveling wave. See Appendix B.1 for the nondimensionalization of the Rayleigh-Plesset Equation.

1.1.2 Translation Equation

The translational dynamics are governed by a balance of linear momentum, detailed by Magnaudet and Legendre [4] and reconsidered by Reddy and Szeri [5]. The equation is

$$\frac{2\pi}{3}\rho\frac{d}{dt}\left(R(t)^3\left(U_a - \dot{X}(t)\right)\right) = \frac{4\pi}{3}R(t)^3\nabla P_\infty - 12\pi\mu R(t)\left(U_a - \dot{X}(t)\right) \tag{1.4}$$

and accounts for drag, added mass, and history forces (which fortunately simplify to the Bjerknes force, $-V\nabla P_\infty$ [5]). The new variable $U_a(t)$ is the translational velocity of the bubble relative to the far-field fluid. The balance of far-field fluid momentum in the acoustic limit lets us re-express this new term as

$$\dot{U}_a \approx -\frac{1}{\rho}\nabla P_\infty \tag{1.5}$$

This cleans up $\dot{U}_a$ terms, but does nothing for U_a terms. Considering U_a a traveling wave of the form $U_a(x/c_l - t)$ lets us integrate both sides of Equation 1.5 and exploit the proportional equivalence of time and spatial derivatives of a traveling waves. This gives us the substitution

$$U_a \approx -\frac{1}{\rho c_l} P_\infty. \tag{1.6}$$

As the temporal variation of the traveling wave is much more significant than the spatial variation, we considered letting c_l be effectively infinite use this significance to simplify the translation equation. However, any term arising from the spatial dependence of the far-field pressure is paired with a gradient operator, which in this one-dimensional case is simply d/dx. Differentiating either traveling wave $U_a = U_a(x/cl - t)$ or $P_\infty = P_\infty(x/cl - t)$ with respect to x produces a c_l in the denominator, and the entire term would disappear if we let $c_l \to \infty$. This would leave us with no means of inducing bubble translation - the initiation of translation depends wholly on a spatial gradient of pressure across the bubble. However, we can consider c_l infinite within the argument of the traveling waves and model them as purely a function of time. This is analogous to claiming that the wave passes by so quickly that any translation of the bubble only introduces a negligible phase lag. The final translation equation then becomes

$$\begin{aligned}\frac{1}{3}\rho R(t)^3 \ddot{X}(t) + \rho R(t)^2 \dot{R}(t)\dot{X}(t) + 6\mu R(t)\dot{X}(t) \\ + \frac{P_o}{\rho c_l}\Big(6\mu R(t)F(t) + \rho R(t)^2 \dot{R}(t)F(t) - \rho R(t)^3 \dot{F}(t)\Big) = 0\end{aligned} \tag{1.7}$$

See Appendix B.2 for the nondimensionalization of the translation equation.

Chapter 2

Calculus of Variations

The calculus of variations is a process by which one can generate differential equations that an extreme solution for a given cost function must satisfy. It is considered a calculus of functionals, as its arguments are not finite-dimensional variables but infinite-dimensional functions. This flexibility makes it a truly powerful optimization technique. However, like any optimization technique, the calculus of variations is only as good as its choice of cost function. The process hinges on the assumption that an extremum of some sort in the scalar valued cost function exists. Trying to find a minimal time is the classic example of a sound choice of cost function with a clear extremum.

The process begins with a choice of independent variable, such as time, t, and a selection of unknown functions of that independent variable; $f_1(t)$, $f_2(t)$ through $f_i(t)$. The overall cost function, J, should then be expressed as the integral of some incremental cost function, I, itself a function of the independent variables, the unknown functions, and their derivatives with respect to the unknown variable. The general form of this cost function is given by

$$J = \int_{t_1}^{t_2} I\left(t, f_1(t), f_2(t), \ldots, f_i(t), \frac{df_1}{dt}, \frac{df_2}{dt}, \ldots, \frac{df_i}{dt}, \ldots, f_1^{(n)}, f_2^{(n)}, \ldots, f_i^{(n)}\right) dt. \tag{2.1}$$

The calculus of variations can also accommodate differential and integral constraints composed of the same arguments as I. The differential constraint $g(t, f_j(t), f_j^{(n)}(t)) = 0$ requires the introduction of the unknown Lagrange multiplier field $\lambda(t)$, and the integral constraint $\int_{t_1}^{t_2} h(t, f_j(t), f_j^{(n)}(t))dt + c = 0$ similarly requires ϕ, giving

$$J = \int_{t_1}^{t_2} (I + \lambda(t)g(t))\, dt + \phi \int_{t_1}^{t_2} h(t)dt, +\phi c$$

and combining the integrals gives us

$$J = \int_{t_1}^{t_2} (I + \lambda(t)g(t) + \phi h(t))\, dt + \phi c = \int_{t_1}^{t_2} I^* dt + \phi c.$$

The masterstroke of the calculus of variations is the concept that all of our unknown functions are variations on the hypothetical optimal function. Each unknown function, $f_i(t)$, can be considered as the sum of the optimal $f_i^{opt}(t)$ and some infinitesimal multiple of a variation $\delta f_i(t)$;

$$f_i(t) \to f_i^{opt}(t) + \epsilon \delta f_i(t) \tag{2.2}$$

Similarly, the higher derivatives of the functions, the Lagrange multiplier field, and our entire cost function all become variations on the optimal solution:

$$f_i^{(n)}(t) \to f_i^{opt(n)}(t) + \epsilon \delta f_i^{(n)}(t)$$

$$\lambda(t) \to \lambda^{opt}(t) + \epsilon \delta \lambda(t)$$

$$J \to J^{opt} + \epsilon \delta J$$

$$\phi \to \phi^{opt} + \epsilon \delta \phi$$

Pushing through these substitutions, we arrive at the following:

$$J = J^{opt} + \epsilon \delta J = \int_{t_1}^{t_2} I^* \left(\epsilon, t, f_i^{opt(n)}, \delta f_i^{(n)} \right) dt$$

We can make no assumptions about the optimal cost, J^{opt}, but we have postulated that it has an extremum at $\epsilon = 0$. Thus, it's derivative with respect to ϵ at $\epsilon = 0$ must be identically zero. Doing so gives us

$$\left. \frac{dJ}{d\epsilon} \right|_{\epsilon=0} = 0 = \delta J = \int_{t_1}^{t_2} \frac{d}{d\epsilon} I^* \left. \left(\epsilon, t, f_i^{opt(n)}, \delta f_i^{(n)} \right) \right|_{\epsilon=0} dt \tag{2.3}$$

Differentiating I^* and evaluating at $\epsilon = 0$ is analogous to linearizing with respect to ϵ about 0. The collection of variational terms (δf_i, $\delta\lambda$ and their derivatives) occurs in linear proportion to ϵ. Consequently, $dI^*/d\epsilon$ is also linear in the sense that any term contains only one variational term, and can be considered as

$$\frac{dI^*}{d\epsilon} = a_{1,0}(t) \cdot \delta f_1(t) + a_{1,1}(t) \cdot \delta f_1^{(1)}(t) + \dots$$
$$+ a_{2,0}(t) \cdot \delta f_2(t) + a_{2,1}(t) \cdot \delta f_2^{(1)}(t) + \dots$$
$$+ a_{\lambda,0}(t) \cdot \delta \lambda(t) + a_{\lambda,1}(t) \cdot \delta \lambda^{(1)}(t) + \dots$$

Integration by parts reduces the differentiated variational terms and produces boundary conditions, leaving

$$\frac{dI^*}{d\epsilon} = b_1(t) \cdot \delta f_1(t) + b_2(t) \cdot \delta f_2(t) + \cdots + b_n(t) \cdot \delta f_n(t) + b_\lambda(t) \cdot \delta\lambda(t)$$

and

$$\delta J = 0 = BC's + \int_{t_1}^{t_2} \frac{dI^*}{d\epsilon} dt$$

Due to the arbitrariness with which the variational terms can be chosen each b_i must be identically 0 for all time, and this produces a set of differential equations of the form $b_i = 0$. These are typically nonlinear differential equations in the unknown functions, and their simultaneous solution to appropriate boundary conditions yields an extremal solution that obeys the given constraints.

2.1 Application

To apply the calculus of variations to this problem we must first, as stated, choose an appropriate cost function. We will seek to maximize the distance, X_{period}, traversed by the bubble in one forcing period for our cost function. We do this by integrating the bubble's translational velocity, $X'(\tau)$ over one period of dimensionless time, from τ_0 to τ_{max}. Our version of Equation 2.1 becomes

$$J = X_{period} = \int_0^{\tau_{max}} X'(\tau) d\tau \tag{2.4}$$

We then append our constraints. We have two differential constraints - the nondimensionalized Rayleigh-Plesset and translation equations (see Appendix B) - and one integral constraint - the L_2-norm of the nondimensional far-field overpressure, $\int_0^{\tau_{max}} \hat{F}^2 d\tau = c$. [1] With these and their Lagrange multipliers, Equation 2.4 becomes:

$$J = \int_0^{\tau_{max}} \left(X'(\tau) + \lambda_1(\tau) \cdot ndRPE(\tau) + \lambda_2(\tau) \cdot ndTE(\tau) + \phi \cdot \hat{F}^2 \right) d\tau + \phi c \tag{2.5}$$

The fully expanded cost function contains the following unknown functions, for which the listed substitutions are used. As the general unknown function only appears prior to this

[1] In forming our Raleigh-Plesset equation in section 1.1.1, we assumed U^2 is not significant. This may seem contradictory with assuming the integral constraint is significant. U^2 is insignificant in comparison to the other terms of the Raleigh-Plesset equation, but the integral constraint considered independetly remains pertinent

solution and the optimal function only afterwards, the 'opt' superscript from Equation 2.2 has been dropped for readability.

$$\begin{aligned}
R(\tau) &\rightarrow R(\tau) + \epsilon \cdot \delta R(\tau) \\
R(\tau) &\rightarrow R'(\tau) + \epsilon \cdot \delta R'(\tau) \\
R''(\tau) &\rightarrow R''(\tau) + \epsilon \cdot \delta R''(\tau) \\
\hat{F}(\tau) &\rightarrow \hat{F}(\tau) + \epsilon \cdot \delta \hat{F}(\tau) \\
\hat{F}'(\tau) &\rightarrow \hat{F}'(\tau) + \epsilon \cdot \delta \hat{F}'(\tau) \\
X'(\tau) &\rightarrow X'(\tau) + \epsilon \cdot \delta X'(\tau) \\
X''(\tau) &\rightarrow X''(\tau) + \epsilon \cdot \delta X''(\tau) \\
\lambda_1(\tau) &\rightarrow \lambda_1(\tau) + \epsilon \cdot \delta \lambda_1(\tau) \\
\lambda_2(\tau) &\rightarrow \lambda_2(\tau) + \epsilon \cdot \delta \lambda_2(\tau) \\
\phi &\rightarrow \phi + \epsilon \cdot \delta \phi
\end{aligned}$$

At this point the cost function has become a long and unwieldy expression. A computer algebra system such as MATHEMATICA is highly recommended for the mathematically simple yet logistically difficult steps that follow. As detailed in Equation 2.3, we differentiate with respect to ϵ and set it equal to 0. Following this we reduce the differentiated variations with integration by parts. Note that $X(\tau)$ does not appear in the cost function or the list of substitutions. Therefore, $X'(\tau)$ does not need to be reduced to $X(\tau)$ via integration by parts, only $X''(\tau)$ to $X'(\tau)$. We finally factor the integrand into six terms, each corresponding to one of the six final variations: $\delta R(\tau)$, $\delta X'(\tau)$, $\delta \hat{F}(\tau)$, $\delta \lambda_1(\tau)$, $\delta \lambda_2(\tau)$, and $\delta \phi$. As the variations themselves are wholly arbitrary, each of the associated factors must equal zero. This principle, along with the collected boundary conditions and integral constraint, produces the seven equations listed in Appendix A.1.

A simultaneous solution to these differential equations that satisfies these boundary conditions will yield the optimal trajectories of the unknown functions. The most important of these is the optimal $\hat{F}(\tau)$, which directly gives the pressure amplitude as a function of time we should apply to achieve maximum bubble translation.

2.2 Interpretation of Equations

An inspection of the resultant equation shows ample evidence of the original equations. The second state equation of Equation A.8 is a reordered collection of the terms of Equations

1.2, 1.3 and associated substitutions. In order of their appearance in Equation A.8, they are:

- The gas pressure contribution from surface tension, the third term of Equation 1.3.
- The compressive effect of atmospheric pressure, the $P_l - P_\infty$ term on the right hand side of Equation 1.2.
- The term due to forcing, also from the right hand side of Equation 1.2
- The term due to deviations from equilibrium gas pressure, the first term of Equation 1.3
- The gas pressure contribution from viscous resistance to motion, the second term of Equation 1.3
- The kinetic energy term of the simplified Rayleigh-Plesset Equation, the second term of Equation 1.2;

This shows that the Rayleigh-Plesset equation survives to govern the radial dynamics, and partially validates the physicality of the equations resulting from the variational process. More directly, the second and fourth state equations of Equation A.8 are clearly the re-arranged nondimensionalized governing equations as seen in Equations B.2 and B.4

2.3 Numerical Solution

A close inspection of Equations A.1-A.5 reveals they can be reformulated as a six-equation system of first order differential equations of the form $\dot{X} = f(X)$. The six states of X would be R,$R' \rightarrow \rho$,X',λ_1,$\lambda_1' \rightarrow L_1$, and λ_2. The equations in Appendix A would be used as follows:

$$
\begin{aligned}
dR/d\tau &= R' \\
dR'/d\tau &= derived\, from\, A.1 \\
d(X')/d\tau &= derived\, from\, A.2 \\
d\lambda_1/d\tau &= L_1 \\
d\lambda_1'/d\tau &= derived\, from\, A.5 \\
d\lambda_2/d\tau &= derived\, from\, A.4
\end{aligned}
\tag{2.6}
$$

Equation A.5 initially appears to contain the four unknowns R'',X'', λ_1'', and λ_2'. These are the derivatives of the four states ρ,X',L_1, and λ_2 - of which we must eliminate three. Fortunately Equations A.1, A.2 and A.4 can be can be solved for R'', X'', and λ_2' respectively, which both provides three state equations and allows A.5 to be solved for the fourth. Equation A.3 and its derivative are used to replace any occurrence of $\hat{F}(\tau)$ or $\hat{F}'(\tau)$.

Unfortunately it is not a matter of simply choosing initial conditions for this system and integrating forwards - this method has a host of problems. The most straightforward solution to the boundary conditions are a periodic set for all six states. Posing this as an initial value problem creates a six-dimensional shooting scenario, which is high impractical and undesirable. Also, the derived state equations do not contain the integral constraint integrated quantity c - we are only left with indirect control via the associated Lagrange multiplier, ϕ. Figure 2.1 below shows many of the flaws of the resulting trajectories. These are not optimal solutions, as they do not satisfy equation A.7, the collected boundary conditions. Additionally, the saturation of $\hat{f}(\tau)$ at a positive values results in two undesired effects. The first of these effects is a negative relative pressure to the bubble's equilibrium state, which leads to unbounded radial growth. The second effect is bulk pressure-driven flow leading to a steady state-translational velocity, precisely what the integral constraint was intended to prevent.

However, there exist other approaches that seem promising. Posing the search for a solution as a continuation problem might allow us to approach the solution we cannot reach directly by taking a step-by-step manner. The continuation package AUTO [1] is fully capable of finding solutions to dynamic systems with both integral constraint and periodic boundary condition problems. The principle prerequisite for a continuation problem is to begin at a fixed point, which highlights another problem: there does not seem to be a fixed point for the system posed in Appendix A.2. This can be quickly seen by inspecting the initial version of Equation A.4, derived from the coefficients of $\delta X'$:

$$1 + 36\,\lambda_2(\tau) + 10\,Re\,R(\tau)\,\lambda_2(\tau)\,R'(\tau) + 2\,Re\,R(\tau)^2\,\lambda_2'(\tau) = 0 \tag{2.7}$$

A steady state solution to this equation clearly requires a nonzero $\lambda_2(\tau)$, which in turn excites $\hat{F}\tau$ as seen in Equation A.3, which in turn eventually excites all other states. Trying to find a fixed point for the system inevitably leads to a contradictory expressions for one of the two Lagrange multipliers - which is unacceptable. The system is derived from a physical system that clearly has an equilibrium state, yet the system produced by the calculus of variations is self-exciting - in another word, unstable. This effect must be due to

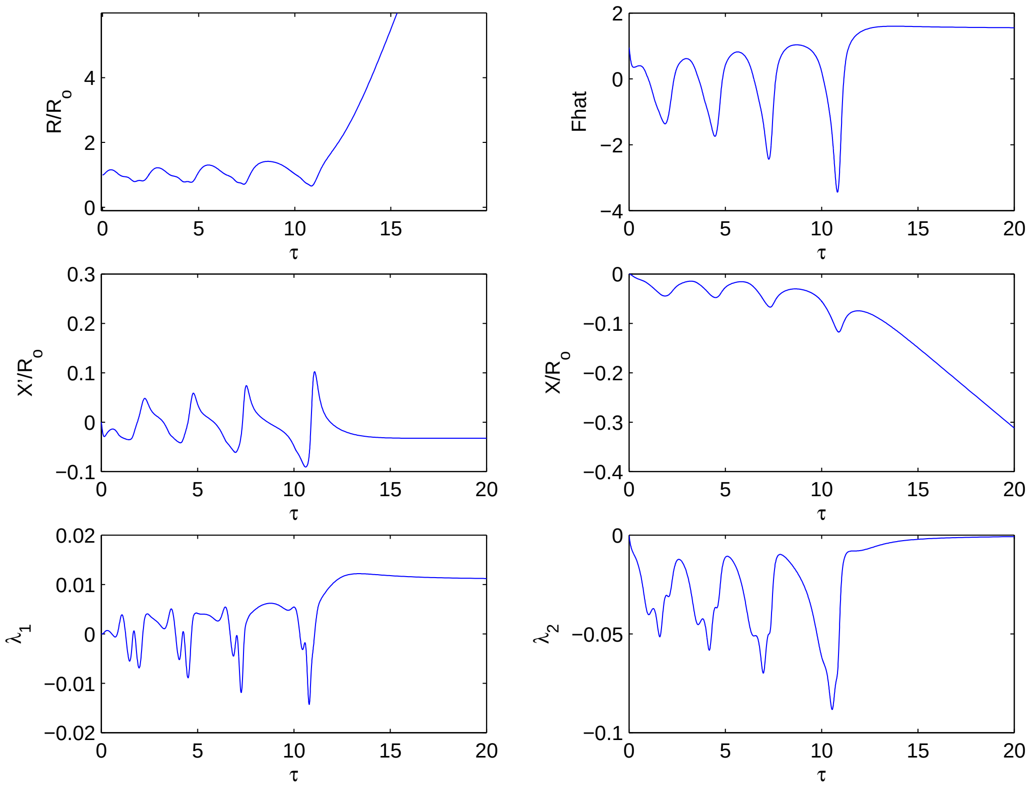

Figure 2.1. Typical initial value problem formulation output. $\phi = 0.032$, R(0) = 1, all other intial conditions zero

the unphysical element of the variational process, the cost function. Indeed, the constant term in Equation 2.7 is due to the $X'(\tau)$ of Equation 2.4. Modifying Equation 2.4 with a multiplicative parameter η gives us

$$J = \eta X_{period} = \int_0^{\tau_{max}} \eta X'(\tau) d\tau$$

The sole effect of pushing this through the calculus of variations is a modified Equation 2.7:

$$\eta + 36\,\lambda_2(\tau) + 10\,Re\,R(\tau)\,\lambda_2(\tau)\,R'(\tau) + 2\,Re\,R(\tau)^2\,\lambda_2'(\tau) = 0 \tag{2.8}$$

Starting with $\eta = 0$ permits a quiescent solution to the system, with $R(0) = 1$ and all other initial conditions zero. The continuation algorithm fails when initially trying to continue from $\eta = 0$ to $\eta = 1$, which suggests the necessity for a less direct approach. Exciting the system via homotopy - an artificially introduced forcing to make the system depart the fixed point - has proven promising in similar problems. The homotopy is the parent's hand that lets the child learn to ride it's bicycle - and when the homotopic forcing is removed, the excited system can hopefully be continued to an unmodified solution to the original equations.

Chapter 3

Conclusions

We have arrived at a system of equations whose solution must be the optimal trajectories for an acoustically forced bubble, subject to the coupled radial and translation dynamics modeled. The attempts to date to solve these equations have failed, but there are thus far promising results. AUTO has been used to simulate a bubble's response to arbitrary forcing scaled by the continuation parameter. These solutions agree to machine precision with more traditional numerical simulation methods. We have yet to successfully tease a response out of the full system of equation, but have a promising continuation algorithm. Given four parameters - η, the cost weighting parameter, α, the homotopy parameter, c, the integral cost, and ϕ, the integral Lagrange multiplier:

- Holding η at zero, continue in the direction of increasing α, leave c free. Let ϕ float if necessary.
- Given an excited solution, continue in the direction of increasing η, to $\eta = 1$, also letting c float.
- With $\eta = 1$, reduce α, removing the artificial forcing, while holding c and letting ϕ float.
- Vary c while allowing ϕ to float, and explore the solution space.

The bulk of the current difficulties lie in satisfying the periodic boundary conditions required under the homotopic forcing. It is possible that a naive choice for forcing - such as the sinusoids used thus far - may be insufficient. Further investigation will hopefully lead to techniques that will solve this problem, and enable the solution of a larger class of similar problems.

Appendix A

Final Equations

A.1 Variational Coefficients

The final cost functional can be grouped into five terms, each with one variational term. Due to the arbitrariness of the individual variational terms, the coefficient for each term must be identically zero, giving rise to the following six-equation integro-differential-algebraic system and associated boundary conditions.

$\delta\lambda_1$:

$$\frac{-4}{We\,R(\tau)} - \frac{P_o^*}{2} + \frac{\hat{F}(\tau)\,P_o^*}{2} + \frac{\left(\frac{1}{R(\tau)}\right)^{3\,k} P_{go}^*\,P_o^*}{2} - \frac{4\,R'(\tau)}{Re\,R(\tau)} - \frac{3\,R'(\tau)^2}{2} - R(\tau)\,R''(\tau) = 0 \quad \text{(A.1)}$$

$\delta\lambda_2$:

$$18\,\hat{F}(\tau)\,M_l\,P_o^* - 3\,Re\,R(\tau)^2\,M_l\,P_o^*\,\hat{F}'(\tau) + 3\,Re\,\hat{F}(\tau)\,R(\tau)\,M_l\,P_o^*\,R'(\tau) + 36\,X'(\tau) + 6\,Re\,R(\tau)\,R'(\tau)\,X'(\tau) + 2\,Re\,R(\tau)^2\,X''(\tau) = 0 \quad \text{(A.2)}$$

$\delta\hat{F}$:

$$-2\,\phi\,\hat{F}(\tau) + \frac{P_o^*\,\lambda_1(\tau)}{2} + 18\,M_l\,P_o^*\,\lambda_2(\tau) - 3\,Re\,R(\tau)\,M_l\,P_o^*\,\lambda_2(\tau)\,R'(\tau) - 3\,Re\,R(\tau)^2\,M_l\,P_o^*\,\lambda_2'(\tau) = 0 \quad \text{(A.3)}$$

$\delta X'$:

$$\eta + 36\,\lambda_2(\tau) + 10\,Re\,R(\tau)\,\lambda_2(\tau)\,R'(\tau) + 2\,Re\,R(\tau)^2\,\lambda_2'(\tau) = 0 \tag{A.4}$$

δR:

$$\frac{4\,\lambda_1(\tau)}{We\,R(\tau)^2} - \frac{3}{2}\,k\left(\frac{1}{R(\tau)}\right)^{1+3\,k} P_{go}^*\,P_o^*\,\lambda_1(\tau) - 3\,Re\,R(\tau)\,M_l\,P_o^*\,\lambda_2(\tau)\,\hat{F}'(\tau)$$
$$+ \frac{8\,\lambda_1(\tau)\,R'(\tau)}{Re\,R(\tau)^2} + 6\,Re\,\hat{F}(\tau)\,M_l\,P_o^*\,\lambda_2(\tau)\,R'(\tau) + 12\,Re\,\lambda_2(\tau)\,R'(\tau)\,X'(\tau)$$
$$- \frac{4\,\lambda_2'(\tau)}{Re\,R(\tau)} - 5\,R'(\tau)\,\lambda_2'(\tau) + 3\,Re\,\hat{F}(\tau)\,R(\tau)\,M_l\,P_o^*\,\lambda_2'(\tau)$$
$$+ 6\,Re\,R(\tau)\,X'(\tau)\,\lambda_2'(\tau) - 5\,\lambda_1(\tau)\,R''(\tau) + 10\,Re\,R(\tau)\,\lambda_2(\tau)\,X''(\tau)$$
$$- R(\tau)\,\lambda_2''(\tau) = 0 \tag{A.5}$$

Integral Constraint:

$\delta\phi$:

$$\int_0^{\tau_{max}} \hat{F}^2 d\tau = c \tag{A.6}$$

Boundary Conditions:

$$\delta\hat{F}(0)\left(3\,Re\,R(0)^2\,M_l\,P_o^*\,\lambda_2(0)\right) - \delta\hat{F}(\tau_{max})\left(3\,Re\,R(\tau_{max})^2\,M_l\,P_o^*\,\lambda_2(\tau_{max})\right)$$
$$+ \delta R'(0)\Big(R(0)\,\lambda_1(0)\Big) - \delta R'(\tau_{max})\Big(R(\tau_{max})\,\lambda_1(\tau_{max})\Big)$$
$$- \delta X'(0)\left(2\,Re\,R(0)^2\,\lambda_2(0)\right) + \delta X'(\tau_{max})\left(2\,Re\,R(\tau_{max})^2\,\lambda_2(\tau_{max})\right)$$
$$- \delta R(0)\left(\frac{-4\,\lambda_1(0)}{Re\,R(0)} + 3\,Re\,\hat{F}(0)\,R(0)\,M_l\,P_o^*\,\lambda_2(0) - 4\,\lambda_1(0)\,R'(0)\right.$$
$$\left. + 6\,Re\,R(0)\,\lambda_2(0)\,X'(0) - R(0)\,\lambda_2'(0)\right)$$
$$+ \delta R(\tau_{max})\left(\frac{-4\,\lambda_1(\tau_{max})}{Re\,R(\tau_{max})} + 3\,Re\,\hat{F}(\tau_{max})\,R(\tau_{max})\,M_l\,P_o^*\,\lambda_2(\tau_{max}) - 4\,\lambda_1(\tau_{max})\,R'(\tau_{max})\right.$$
$$\left. + 6\,Re\,R(\tau_{max})\,\lambda_2(\tau_{max})\,X'(\tau_{max}) - R(\tau_{max})\,\lambda_2'(\tau_{max})\right) = 0 \tag{A.7}$$

A.2 State Space Representation

The first five equations (A.1 - A.5) above can be realized as a six-state system of first order differential equations. While $\hat{F}$ can be calculated algebraically, it must be differentiated to calculate $\hat{F}'$. Given this value, including it as an additional seventh state is a useful recording tactic. Similarly, introducing an eighth state for $X(\tau)$ implifies the integration of $X'(\tau)$. This yields the following eight-state system:

$$
\begin{aligned}
dR/d\tau =& R'(\tau) \\
dR'/d\tau =& \frac{-4}{We\,R(\tau)^2} - \frac{P_o^*}{2\,R(\tau)} + \frac{\hat{F}(\tau)\,P_o^*}{2\,R(\tau)} + \frac{\left(\frac{1}{R(\tau)}\right)^{1+3\,k} P_{go}^*\,P_o^*}{2} - \frac{4\,R'(\tau)}{Re\,R(\tau)^2} - \frac{3\,R'(\tau)^2}{2\,R(\tau)} \\
dX/d\tau =& X'(\tau) \\
dX'/d\tau =& \frac{-9\,\hat{F}(\tau)\,M_l\,P_o^*}{Re\,R(\tau)^2} + \frac{3\,M_l\,P_o^*\,\hat{F}'(\tau)}{2} - \frac{3\,\hat{F}(\tau)\,M_l\,P_o^*\,R'(\tau)}{2\,R(\tau)} - \frac{18\,X'(\tau)}{Re\,R(\tau)^2} - \frac{3\,R'(\tau)\,X'(\tau)}{R(\tau)} \\
d\lambda_1/d\tau =& \lambda_1'(\tau) \\
d\lambda_1'/d\tau =& \frac{4\,\lambda_1(\tau)}{We\,R(\tau)^3} - \frac{3\,k\left(\frac{1}{R(\tau)}\right)^{2+3\,k} P_{go}^*\,P_o^*\,\lambda_1(\tau)}{2} - 3\,Re\,M_l\,P_o^*\,\lambda_2(\tau)\,\hat{F}'(\tau) \\
& + \frac{8\,\lambda_1(\tau)\,R'(\tau)}{Re\,R(\tau)^3} + \frac{6\,Re\,\hat{F}(\tau)\,M_l\,P_o^*\,\lambda_2(\tau)\,R'(\tau)}{R(\tau)} + \frac{12\,Re\,\lambda_2(\tau)\,R'(\tau)\,X'(\tau)}{R(\tau)} \\
& - \frac{4\,\lambda_2'(\tau)}{Re\,R(\tau)^2} - \frac{5\,R'(\tau)\,\lambda_2'(\tau)}{R(\tau)} + 3\,Re\,\hat{F}(\tau)\,M_l\,P_o^*\,\lambda_2'(\tau) + 6\,Re\,X'(\tau)\,\lambda_2'(\tau) \\
& - \frac{5\,\lambda_1(\tau)\,R''(\tau)}{R(\tau)} + 10\,Re\,\lambda_2(\tau)\,X''(\tau) \\
d\lambda_2/d\tau =& \frac{-\eta}{2\,Re\,R(\tau)^2} - \frac{18\,\lambda_2(\tau)}{Re\,R(\tau)^2} - \frac{5\,\lambda_2(\tau)\,R'(\tau)}{R(\tau)} \\
d\hat{F}/d\tau =& \frac{P_o^*}{4\,\phi}\Big(\lambda_2'(\tau) + 24\,M_l\Big(\left(6 + Re\,R(\tau)\,R'(\tau)\right)\lambda_2'(\tau) \\
& + Re\,\lambda_2(\tau)\left(R'(\tau)^2 + R(\tau)\,R''(\tau)\right)\Big)\Big)
\end{aligned}
\tag{A.8}
$$

The states are listed in the order given for conceptual clarity. The chain of dependencies is such that the following order of evaluation is required: $\lambda_2'(\tau)$, $R''(\tau)$, $\hat{F}'(\tau)$,$X''(\tau)$,$\lambda_1''(\tau)$.

Appendix B

Nondimensionalization of the Governing Equations

B.1 Rayleigh-Plesset Equation

To nondimensionalise the simplified Rayleigh-Plesset Equation 1.2, the following substitutions were used:

$$
\begin{aligned}
R(t) &\rightarrow R_o R(\tau) \\
R'(t) &\rightarrow R_o f_n R'(\tau) \\
R''(t) &\rightarrow R_o f_n^2 R''(\tau) \\
F[x/c_l - t] &\rightarrow \hat{F}(\tau) \\
\sigma &\rightarrow 2\rho \frac{R_o^3 f_n^2}{We} \\
\mu &\rightarrow \rho \frac{R_o^2 f_n}{Re} \\
P_o &\rightarrow \frac{P_o^* \rho R_o^2 f_n^2}{2}
\end{aligned}
$$

Where f_n is the Minnaert resonant frequency of the bubble as derived in Leighton [3], given by

$$f_n = \frac{1}{R_o}\sqrt{\frac{3\gamma P_o}{\rho}} \tag{B.1}$$

Under these substitutions, the nondimensionalized RPE is

$$\frac{4}{We\,R(\tau)} + \frac{P_o^*}{2} - \frac{\hat{F}(\tau)\,P_o^*}{2} - \frac{\left(\frac{1}{R(\tau)}\right)^{3\,k} P_{go}^*\,P_o^*}{2} + \frac{4\,R'(\tau)}{Re\,R(\tau)} + \frac{3\,R'(\tau)^2}{2} + R(\tau)\,R''(\tau) = 0 \quad \text{(B.2)}$$

B.2 Translation Equation

To nondimensionalise the simplified translation equation 1.4, the following substitutions were used:

$$\begin{aligned}
R(t) &\to R_o R(\tau) \\
R'(t) &\to R_o f_n R'(\tau) \\
F[x/c_l - t] &\to \hat{F}(\tau) \\
F'[x/c_l - t] &\to f_n \hat{F}'(\tau) \\
X'(t) &\to R_o f_n X'(\tau) \\
X''(t) &\to R_o f_n^2 X''(\tau) \\
\mu &\to \rho \frac{R_o^2 f_n}{Re} \\
P_o &\to \frac{P_o^* \rho R_o^2 f_n^2}{2} \\
c_l &\to \frac{R_o f_n}{M_l}
\end{aligned} \quad \text{(B.3)}$$

Where f_n is the same Minnaert resonant frequency used above. These substitutions yield the final nondimensional translation equation

$$- 18\,\hat{F}(\tau)\,M_l\,P_o^* + 3\,Re\,R(\tau)^2\,M_l\,P_o^*\,\hat{F}'(\tau) - 3\,Re\,\hat{F}(\tau)\,R(\tau)\,M_l\,P_o^*\,R'(\tau) - 36\,X'(\tau) - 6\,Re\,R(\tau)\,R'(\tau)\,X'(\tau) - 2\,Re\,R(\tau)^2\,X''(\tau) = 0 \quad \text{(B.4)}$$

Appendix C

Variables and Parameters

Variables

Symbol	*VariableName*
t	Time
τ	Nondimensional time, t/f_n
$R(t), \dot{R}(t), \ddot{R}(t)$	Bubble radial position and derivatives
$R(\tau), R'(\tau), R''(\tau)$	Nondimensional bubble radial position and derivatives
$X(t), \dot{X}(t), \ddot{X}(t)$	Bubble translational position and derivatives
$X(\tau), X'(\tau), X''(\tau)$	Nondimensional bubble translational position and derivatives
$F(t), \hat{F}(\tau)$	Far-field overpressure term (positive F $\rightarrow$ negative pressure)
$\lambda_1(\tau), \lambda_1(\tau)', \lambda_1(\tau)''$	RPE Lagrange multiplier field and derivatives
$\lambda_2(\tau), \lambda_2(\tau)'$	Translation Eq. Lagrange multiplier field and derivatives
ϕ	Integral constraint Lagrange multiplier
η	Cost weighting

Parameters

Symbol	*Quantity*	*TypicalNumericalValue*
R_o	Initial bubble radius	$2e{-}6$ $[m]$
f_n	Bubble resonant frequency	$1.68e6$ $[s^{-1}]$
σ	Liquid surface tension	0.0728 $[Nm^{-1}]$
ρ	Liquid density	998 $[kgm^{-3}]$
μ	Liquid viscosity	0.001 $[Nsm^{-2}]$
c_l	Speed of sound in liquid	1484.7 $[ms^{-1}]$
P_o	Atmospheric Pressure	101325 $[Nm^{-2}]$
Re	Reynolds number	6.71
We	Weber number	0.619
M_l	'Mach' number in the fluid	2.26e-3
P^*_{go}	Nondimensional initial gas pressure	1.72
P^*_o	Pressure nondimensionalization coefficient	17.99

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