GPU Accelerated Four Dimensional Parameter Scan of a Dual-Frequency Driven Single Gas Bubble

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Sonochemistry is the promotion of chemical reactions in liquid phase by strong ultrasound fields where the key phenomenon is the acoustic cavitation and the collapse of the emerging bubbles. A promising technique that has recently drawn the attention of researchers is the use of a second ultrasonic driving frequency to increase the chemical yield. Due to the large involved parameter space even in a single spherical bubble, clear theoretical understanding is still missing, see e.g. the paper of Rahimi et al. [1] about the advantages and disadvantages of the application of dual-frequency driving.

A good strategy to resolve this discrepancy is to employ a bottom-up approach. That is, investigate the simplest but still suitable model first in which a huge parameter scan can be easily obtained. Then gradually increase the complexity of the model and perform further simulations based on the experience of the previous results until a good theoretical explanation is found. Having done the initial step, the main aim in this study is to present numerical simulations obtained by solving the Keller—Miksis equation well known in sonochemistry that is a simple second order ordinary differential equation describing the dynamics of a single spherical gas bubble [2].

The investigated four dimensional parameters space is composed by the properties of the dual-frequency driving: amplitudes (P_{A1}, P_{A2}) varied between 0 and 2 bar; frequencies normalized by the linear undamped eigenfrequency of the system (ω_{R1}, ω_{R2}) spanned in the range 0.1 and 10. Even with a moderate resolution of 100 values of each parameters applied here (the effect of phase angle is neglected, the equilibrium bubble size is $10\ \mu\mathrm{m}$), one hundred million transient initial value problems have to be solved. The initial condition is the equilibrium state of the unexcited system at each parameter combination. In order to obtain results of such very detailed analysis within reasonable time, the high computational capacities of professional GPUs were exploited (2 Nvidia Tesla K20m). The overall computations took approximately one week. The integration algorithm was the adaptive Runge–Kutta–Cash–Karp method.

After the initial transient (1024 number of collapses), 64 additional collapses were simulated and saved their properties (maximum and minimum bubble radii, collapse times and maximum bubble wall velocities). A collapse is defined as the evolution of the bubble radius from a local maximum to a subsequent local minimum. The above quantities provide a good flexibility to describe the strength of a bubble collapse mandatory for efficient application. The data of the 64 number of collapses allows to make a coarse statistical investigation as well. In addition, the total

time of the 64 collapses were also recorded, which makes it possible to determine the number of the strong collapses (a suitable threshold is required) in a unit time. The overall size of the collected data is approximately 350 GB. In the present paper, we focus only in the examination of the **maximum bubble radius** used also by many researchers [3, 4].

The main difficulty is the presentation of the results in the 4D parameter space. As a first step, bi-parametric contour plots of the maximum bubble radius were created in the plane of the relative frequencies at fixed pressure amplitudes. Out of the $100 \times 100 = 10000$ plots, only one is presented in the left hand side of **Fig. 1** at $P_{A1} = 0.6$ bar and $P_{A2} = 0.8$ bar. The vertical and horizontal light blue stripes indicate the main, harmonic and the first subharmonic resonances. It is clear that high maximum bubble radius can be achieved only at low frequencies (red-yellow domain). This low frequency region is known as the giant response region. Taking the highest value of the maximum bubble radii at every bi-parametric plots, a condensed representation of the achievable collapse strengths can be obtained as a function of the pressure amplitudes, see **Fig. 1** right. The value at the cross (56.7 μm) corresponds to the highest maximum bubble radius in the plane of the frequencies shown in **Fig. 1** left.

The diagonal isolines in the right hand side of **Fig. 1** indicate that the collapse strength in terms of the maximum bubble radius is governed exclusively by the algebraic sum of the individual amplitudes. Therefore, the evolution of **the maximum bubble radius cannot explain the high increase** (sometimes 300% [5]) **of the efficacy of sonochemistry** compared to single-frequency driving. Since only the maximum value of the excitation is important, the only optimization possible is the distribution of power between the ultrasonic transducers (best if equal). These results call the main outcome some previous studies [3, 4] into the question. Consequently, other explanation(s) need to be found and investigated in more details. Some possible candidates: other measures for the strength of the collapse and/or the number of strong collapse in a unit time may show different trends; dual frequency may stabilize the spherical shape of the bubbles; or the efficiency increase maybe inherently due to the collective dynamics of bubbles in a cluster.

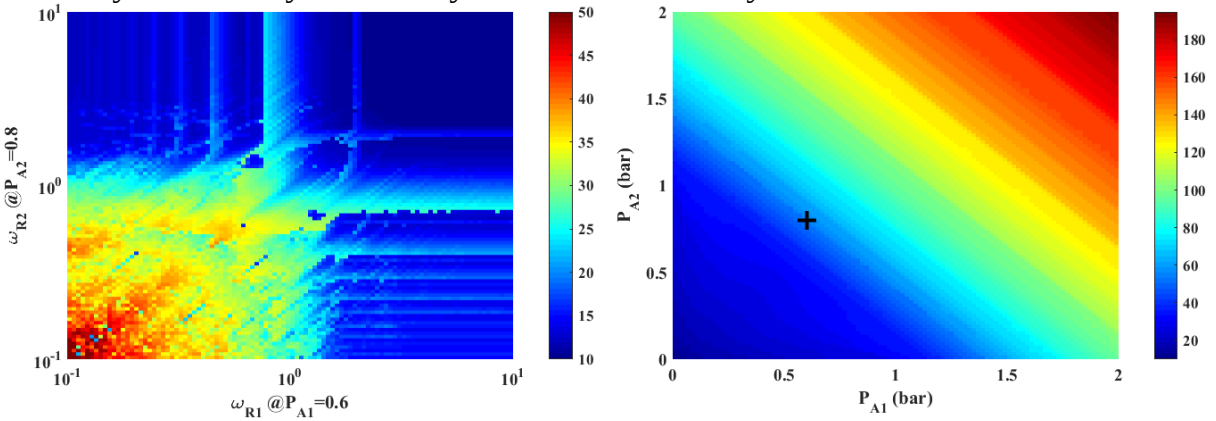

Figure 1. Left panel: Maximum bubble radii as a function of the relative frequencies ω_{R1} and ω_{R2} at pressure amplitudes $P_{A1} = 0.6$ bar and $P_{A2} = 0.8$ bar. Right: Achievable maximum bubble radius as a function of the pressure amplitudes. The equilibrium bubble radius $R_E = 10$ μm.

References

[1] Rahimi M., Safari S., Faryadi M., Moradi N. et al. *Chem. Eng. Process.*, 78: 17-26. **2014.**
[2] Lauterborn W., Kurz T. *Rep. Prog. Phys.*, 73: 106501. **2010.**
[3] Guédra M., Inserra C., Gilles B. et al. *Ultrason. Sonochem*, 38: 298-305. **2017.**
[4] Zhang Y., Zhang Y., Li S. et al. *Ultrason. Sonochem*, 35: 431-439. **2017.**
[5] Wang M., Zhou Y. *Ultrason. Sonochem*, 42: 327-338. **2018.**

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