On the Modeling and Simulation of a Laser-Induced Caviation Bubble

Ali Zein

Supervisor: Prof. Dr. Gerald Warnecke
Co-supervisor: Dr. Maren Hantke

Institut für Analysis und Numerik
Otto-von-Guericke-Universität Magdeburg

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Outline of Topics

1. Introduction
2. Mathematical Model
3. Mathematical Properties of the Model
4. Numerical Method
   - Hyperbolic Operator
   - Source and Relaxation Operators
   - Temperature Relaxation
5. Numerical Results
6. Future Work

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Introduction

- The aim of this work is to present numerical investigations for the collapse and rebound of a laser-induced cavitation bubble in a compressible fluid.
- The Saurel and Abgrall model for two phase flow [1] is used, with a modification for the volume fraction equation.
- The phase velocities, pressures and temperatures will relax to a common value.
- We introduced a procedure for the temperature relaxation that is used at each time step after the pressure relaxation, we used the fact that mechanical properties relax much faster than the thermal properties.

[1] R. Saurel , R. Abgrall, A multiphase Godunov method for compressbile multifluid and multiphase flows, Journal of Computational Physics, 150 (2), 425-467, (1999).

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The model in spherical coordinates assuming rotational symmetry, with a modification for the volume fraction equation can be written as

$$\frac{\partial \alpha_1}{\partial t} + U\frac{\partial \alpha_1}{\partial r} = \mu(p_1 - p_2) + \frac{\theta}{\Phi}(T_1 - T_2) \tag{1a}$$

$$\frac{\partial \alpha_1\rho_1}{\partial t} + \frac{\partial(\alpha_1\rho_1 u_1)}{\partial r} = \frac{-2}{r}\alpha_1\rho_1 u_1 \tag{1b}$$

$$\frac{\partial \alpha_1\rho_1 u_1}{\partial t} + \frac{\partial(\alpha_1\rho_1 u_1^2 + \alpha_1 p_1)}{\partial r} = P\frac{\partial \alpha_1}{\partial r} + \lambda(u_2 - u_1) - \frac{2}{r}\alpha_1\rho_1 u_1^2 \tag{1c}$$

$$\begin{aligned}\frac{\partial \alpha_1\rho_1 E_1}{\partial t} + \frac{\partial((\rho_1 E_1 + p_1)\alpha_1 u_1)}{\partial r} &= PU\frac{\partial \alpha_1}{\partial r} + \mu P(p_2 - p_1) \\ &\quad + \lambda U(u_2 - u_1) + \theta(T_2 - T_1) - \frac{2}{r}((\rho_1 E_1 + p_1)\alpha_1 u_1)\end{aligned} \tag{1d}$$

$$\frac{\partial \alpha_2\rho_2}{\partial t} + \frac{\partial(\alpha_2\rho_2 u_2)}{\partial r} = \frac{-2}{r}\alpha_2\rho_2 u_2 \tag{1e}$$

$$\frac{\partial \alpha_2\rho_2 u_2}{\partial t} + \frac{\partial(\alpha_2\rho_2 u_2^2 + \alpha_2 p_2)}{\partial r} = -P\frac{\partial \alpha_1}{\partial r} - \lambda(u_2 - u_1) - \frac{2}{r}\alpha_2\rho_2 u_2^2 \tag{1f}$$

$$\begin{aligned}\frac{\partial \alpha_2\rho_2 E_2}{\partial t} + \frac{\partial((\rho_2 E_2 + p_2)\alpha_2 u_2)}{\partial r} &= -PU\frac{\partial \alpha_1}{\partial r} - \mu P(p_2 - p_1) \\ &\quad - \lambda U(u_2 - u_1) - \theta(T_2 - T_1) - \frac{2}{r}((\rho_2 E_2 + p_2)\alpha_2 u_2)\end{aligned} \tag{1g}$$

The notations are classical:

α_k : The volume fraction $(\alpha_1 + \alpha_2 = 1)$
ρ_k : The density.
u_k : The radial velocity.
p_k : The pressure.
T_k : The temperature.
$E_k = e_k + \frac{u_k^2}{2}$: The total specific energy, where e_k is the specific internal energy.

Interfacial variables

P and U are the interfacial pressure and interfacial velocity respectively.

$$P = \sum_{k=1}^{2} \alpha_k p_k, \qquad U = \sum_{k=1}^{2} \frac{\alpha_k \rho_k u_k}{\alpha_k \rho_k} \tag{2}$$

Relaxation parameters

The parameters λ, μ and $\theta > 0$ are the relaxation parameters which determine the rates at which the velocities, pressures and temperatures of the two phases relax to a common value.

Our modification

We added the last term in the equation of volume fraction (1a).

The new variable Φ has to be determined.

Our assumptions

We assume that:

- The relaxation time is very small compared with the other characteristic times
- The pressure relaxation time is much smaller than that of temperature. This assumption agrees with physical evidence in a large number of situations [2].

[2] H. Guillard and M. Labois, Numerical modelling of compressible two-phase flows, European Conference on Computational Fluid Dynamics ECCOMAS CFD 2006, P. Wesseling and E. Onate and J. Priaux (Eds), 2006.

Equations of State (EOS)

To overcome the problem of negative squares of sound speed in numerical computations, each fluid obeys its own EOS as a pure material, also these EOS should satisfy certain convexity constraints.

- Stiffened gas EOS are used for their simplicity, they are expressed as

$$e_k = \frac{p_k + \gamma_k \pi_k}{\rho_k(\gamma_k - 1)}, \qquad k = 1, 2. \tag{3}$$

- Assuming that phase "1" is water vapor and phase "2" liquid water, the closure relations for temperatures can be given as

$$T_1 = \frac{p_1 + \gamma_1 \pi_1}{C_{v1}\rho_1(\gamma_1 - 1)}, \qquad T_2 = \frac{e_2 - \frac{\gamma_2 \xi}{\rho_2}}{C_{v2}} + T_0 \tag{4}$$

Phase	γ	$\pi(Pa)$	$C_v(J/kg/K)$	$\xi(Pa)$	$T_0(K)$
1	1.327	0	1.41×10^3	-	-
2	4.4	6.6×10^7	4.2×10^3	6.0×10^5	273.15

Table 1: EOS parameters for vapor and liquid water

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Mathematical Properties of the Model

The model (1) in terms of primitive variables can be written as

$$\frac{\partial \mathbf{W}}{\partial t} + \mathbf{A}\frac{\partial \mathbf{W}}{\partial r} = \mathbf{S} \tag{5}$$

where $\mathbf{W} = (\alpha_1, \rho_1, u_1, p_1, \rho_2, u_2, p_2)^T$, the source vector $\mathbf{S}$ represents the non-differential source terms.

The eigenvalues are

$$\begin{aligned} &\lambda_1 = U, \\ &\lambda_2 = u_1 - c_1, \quad \lambda_3 = u_1, \quad \lambda_4 = u_1 + c_1, \\ &\lambda_5 = u_2 - c_2, \quad \lambda_6 = u_2, \quad \lambda_7 = u_2 + c_2. \end{aligned} \tag{6}$$

- The system is hyperbolic.
- Considering the Riemann problem of the system:
  - The 1-, 3- and 6- fields are linearly degenerate.
  - The 2-, 4-, 5- and 7- fields are genuinely nonlinear.

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Numerical Method

To account for hyperbolic part and non-differentiable source terms we use the Strang splitting approach [3]. Thus the solution is obtained by the succession of operators

$$\mathbf{U}_j^{n+1} = L_s^{\frac{\Delta t}{2}} L_h^{\Delta t} L_s^{\frac{\Delta t}{2}} \mathbf{U}_j^n \tag{7}$$

where
$\mathbf{U} = (\alpha_1, \alpha_1\rho_1, \alpha_1\rho_1 u_1, \alpha_1\rho_1 E_1, \alpha_2\rho_2, \alpha_2\rho_2 u_2, \alpha_2\rho_2 E_2)^T$.

$L_h^{\Delta t}$ is the operator of numerical solution of the hyperbolic part of the system (1) over Δt

$L_s^{\frac{\Delta t}{2}}$ is the operator of integration of the source and relaxation terms over half of the time interval, i.e. $\dfrac{\Delta t}{2}$.

[3] G. Strang, On the construction and comparison of difference schemes, SIAM J. Num. Anal. 5, 506-517 (1968).

Hyperbolic Operator

- A modified Godunov type scheme is used to take into account the discretization of non-conservative part of the system.
- The discretization of non-conservative terms depends on the choice of the flux for the conservative fluxes.
- HLL and HLLC solvers are used.
- To achieve second order accuracy the **MUSCL** method is used.

Source and Relaxation Operators

- According to the Strang splitting (7), we have to solve the following system of ordinary differential equations.

$$\frac{d\mathbf{U}}{dt} = \mathbf{S} \tag{8}$$

where $\mathbf{U} = (\alpha_1, \alpha_1\rho_1, \alpha_1\rho_1 u_1, \alpha_1\rho_1 E_1, \alpha_2\rho_2, \alpha_2\rho_2 u_2, \alpha_2\rho_2 E_2)^T$

- The source vector $\mathbf{S}$ can be decomposed as

$$\mathbf{S} = \mathbf{S}_S + \mathbf{S}_V + \mathbf{S}_P + \mathbf{S}_T \tag{9}$$

where $\mathbf{S}_V, \mathbf{S}_P$ and $\mathbf{S}_T$ are associated with velocity, pressure and temperature relaxation terms respectively and $\mathbf{S}_S$ represents the other source terms.

$$\mathbf{S}_S = \begin{bmatrix} 0 \\ -2\alpha_1\rho_1 u_1/r \\ -2\alpha_1\rho_1 u_1^2/r \\ -2((\rho_1 E_1 + p_1)\alpha_1 u_1)/r \\ -2\alpha_2\rho_2 u_2/r \\ -2\alpha_2\rho_2 u_2^2/r \\ -2((\rho_2 E_2 + p_2)\alpha_2 u_2)/r \end{bmatrix}, \quad \mathbf{S}_V = \begin{bmatrix} 0 \\ 0 \\ \lambda(u_2 - u_1) \\ \lambda U(u_2 - u_1) \\ 0 \\ -\lambda(u_2 - u_1) \\ -\lambda U(u_2 - u_1) \end{bmatrix}, \quad (10)$$

$$\mathbf{S}_P = \begin{bmatrix} \mu(p_1 - p_2) \\ 0 \\ 0 \\ \mu P(p_2 - p_1) \\ 0 \\ 0 \\ -\mu P(p_2 - p_1) \end{bmatrix} \quad \text{and} \quad \mathbf{S}_T = \begin{bmatrix} \frac{\theta}{\Phi}(T_2 - T_1) \\ 0 \\ 0 \\ \theta(T_2 - T_1) \\ 0 \\ 0 \\ -\theta(T_2 - T_1) \end{bmatrix} \quad (11)$$

- The system (8) is solved by successive integrations considering each one of the source vectors alone.
- The solution of the system (8) with $\mathbf{S}_S$ can be achieved by e.g. Runge-Kutta schemes.
- The system (8) with velocity and pressure relaxation terms is solved by instantaneous relaxation procedures of Saurel and Abgrall [1].

[1] R. Saurel , R. Abgrall, A multiphase Godunov method for compressbile multifluid and multiphase flows, Journal of Computational Physics, 150 (2), 425-467, (1999).

Temperature Relaxation

In order to have a temperature relaxation we solve the following system of ODE

$$\frac{d\mathbf{U}}{dt} = \mathbf{S}_T \tag{12}$$

with $\theta \to \infty$.
Consider the equations of phase '1'

$$\frac{\partial \alpha_1}{\partial t} = \frac{\theta}{\Phi}(T_1 - T_2) \tag{13a}$$

$$\frac{\partial \alpha_1 \rho_1}{\partial t} = 0 \tag{13b}$$

$$\frac{\partial \alpha_1 \rho_1 u_1}{\partial t} = 0 \tag{13c}$$

$$\frac{\partial \alpha_1 \rho_1 E_1}{\partial t} = \theta(T_2 - T_1) \tag{13d}$$

- $\alpha_1\rho_1$ and $\alpha_1\rho_1 u_1$ stay constant through the relaxation process.
- From system (13) we can get

$$\frac{\partial e_1}{\partial t} = -\frac{\Phi}{\alpha_1\rho_1}\frac{\partial \alpha_1}{\partial t} \tag{14}$$

- Integrating this equation, we obtain the following approximation

$$e_1^* = e_1^0 - \frac{\bar{\Phi}}{\alpha_1\rho_1}(\alpha_1^* - \alpha_1^0) \tag{15}$$

  where '0' and '*' refer to the states before and after relaxation process and $\bar{\Phi}$ is the mean value between states $(\alpha_1^0, \rho_1^0, e_1^0)$ and $(\alpha_1^*, \rho_1^*, e_1^*)$.
- We can proceed in the same way to get a similar result for phase '2'.
- Now, we aim to find α_1 that satisfy the equilibrium condition

$$g(\alpha_1) = T_2(e_2, \rho_2) - T_1(e_1, \rho_1) = 0 \tag{16}$$

- The temperature relaxation procedure is used at each time step after the pressure relaxation.

- But, now we see that the pressure will change again and we lose the equality of pressure that achieved by the pressure relaxation.

To solve this problem we assume that the pressure will stay constant through the temperature relaxation. This assumption agrees with the physical situation since the pressure relaxed much faster than the temperature.

- It remains to find an appropriate expression for Φ. To do that we use the second law of thermodynamics. i.e. the generated entropy of the mixture increases or stays constant.
- During the temperature relaxation we assume that the velocity and pressure equilibrium conditions are satisfied. To take into account this point, we use the model of one velocity and one pressure. Thus to find Φ we used the entropy equations of a five-equation reduced model.

Applying the reduction method presented in Murrone and Guillard [4] on the model (1), we obtain the following five-equation model

$$\frac{\partial \alpha_1}{\partial t} + \mathbf{u}\cdot\nabla\alpha_1 = \frac{\alpha_1\alpha_2(\rho_2 c_2^2 - \rho_1 c_1^2)}{\alpha_2\rho_1 c_1^2 + \alpha_1\rho_2 c_2^2}\nabla\cdot\mathbf{u} + \frac{\alpha_1\alpha_2(\frac{\Gamma_1}{\alpha_1} + \frac{\Gamma_2}{\alpha_2})}{\alpha_2\rho_1 c_1^2 + \alpha_1\rho_2 c_2^2}(1 - \frac{p}{\Phi})\theta(T_2 - T_1) \tag{17a}$$

$$\frac{\partial \alpha_1\rho_1}{\partial t} + \nabla\cdot(\alpha_1\rho_1\mathbf{u}) = 0 \tag{17b}$$

$$\frac{\partial \alpha_2\rho_2}{\partial t} + \nabla\cdot(\alpha_2\rho_2\mathbf{u}) = 0 \tag{17c}$$

$$\frac{\partial \rho\mathbf{u}}{\partial t} + \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u}) + \nabla p = 0 \tag{17d}$$

$$\frac{\partial \rho E}{\partial t} + \nabla\cdot(\rho E + p)\mathbf{u} = 0 \tag{17e}$$

where $\rho = \alpha_1\rho_1 + \alpha_2\rho_2$, $\rho e = \alpha_1\rho_1 e_1 + \alpha_2\rho_2 e_2$ and $\Gamma_k = \frac{1}{\rho_k}\left(\frac{\partial p_k}{\partial e_k}\right)_{\rho_k}$

[4] A. Murrone, H. Guillard, A five equation reduced model for compressible two phase flow problems, Journal of Computational Physics, 202 (2), 664 - 698 (2005).

To find the entropy equations we proceed in a similar way to the method that used by Saurel, Petitpas and Abgrall [5]. We derive two hybrid equations for the entropies of phases:

- The first equation comes from the using of Gibbs relations with mixture energy and momentum conservation.
- The second equation comes from the pressure equilibrium between phases.

Denote the material derivative as $\frac{D(.)}{Dt} = \frac{\partial(.)}{\partial t} + \mathbf{u} \cdot \nabla(.)$

The Gibbs relation for each phase can be written as

$$T_k ds_k = de_k - \frac{p_k}{\rho_k^2} d\rho_k, \qquad k = 1, 2 \tag{18}$$

where s_k is the specific entropy.

[5] R. Saurel, F. Petitpas and R. Abgrall, Modelling phase transition in metastable liquids: application to cavitating and flashing flows, Journal of Fluid Mechanics, 607, 313-350 (2008).

- Using Gibbs relations with model (17) we obtain

$$\alpha_1 \rho_1 T_1 \frac{Ds_1}{Dt} + \alpha_2 \rho_2 T_2 \frac{Ds_2}{Dt} = 0 \tag{19}$$

- A second equation is derived from the pressure equilibrium

$$p_1(\rho_1, s_1) = p_2(\rho_2, s_2) \tag{20}$$

By differentiation, we have

$$\left(\frac{\partial p_1}{\partial \rho_1}\right)_{s_1} \frac{D\rho_1}{Dt} + \left(\frac{\partial p_1}{\partial s_1}\right)_{\rho_1} \frac{Ds_1}{Dt} = \left(\frac{\partial p_2}{\partial \rho_2}\right)_{s_2} \frac{D\rho_2}{Dt} + \left(\frac{\partial p_2}{\partial s_2}\right)_{\rho_2} \frac{Ds_2}{Dt} \tag{21}$$

Using the following relations for square speed of sound and Gruneisen coefficient

$$c_k^2 = \left(\frac{\partial p_k}{\partial \rho_k}\right)_{s_k}, \qquad \Gamma_k = \frac{1}{\rho_k T_k}\left(\frac{\partial p_k}{\partial s_k}\right)_{\rho_k}, \qquad k = 1, 2 \tag{22}$$

we obtain

$$\rho_1 T_1 \Gamma_1 \frac{Ds_1}{Dt} - \rho_2 T_2 \Gamma_2 \frac{Ds_2}{Dt} = -c_1^2 \frac{D\rho_1}{Dt} + c_2^2 \frac{D\rho_2}{Dt} \tag{23}$$

Using (19) and (23), we get

$$\alpha_1\alpha_2\rho_1 T_1 \left(\frac{\Gamma_1}{\alpha_1} + \frac{\Gamma_2}{\alpha_2}\right) \frac{Ds_1}{Dt} = \alpha_2 \left(c_2^2 \frac{D\rho_2}{Dt} - c_1^2 \frac{D\rho_1}{Dt}\right) \tag{24a}$$

$$\alpha_1\alpha_2\rho_2 T_2 \left(\frac{\Gamma_1}{\alpha_1} + \frac{\Gamma_2}{\alpha_2}\right) \frac{Ds_2}{Dt} = \alpha_1 \left(c_1^2 \frac{D\rho_1}{Dt} - c_2^2 \frac{D\rho_2}{Dt}\right) \tag{24b}$$

with (17b) and (17c) we obtain

$$\alpha_1\rho_1 T_1 \left(\frac{\Gamma_1}{\alpha_1} + \frac{\Gamma_2}{\alpha_2}\right) \frac{Ds_1}{Dt} = \left(\left(\frac{\rho_1 c_1^2}{\alpha_1} + \frac{\rho_2 c_2^2}{\alpha_2}\right) \frac{D\alpha_1}{Dt} - (\rho_2 c_2^2 - \rho_1 c_1^2)\nabla \cdot \mathbf{u}\right) \tag{25a}$$

$$\alpha_2\rho_2 T_2 \left(\frac{\Gamma_1}{\alpha_1} + \frac{\Gamma_2}{\alpha_2}\right) \frac{Ds_2}{Dt} = -\left(\left(\frac{\rho_1 c_1^2}{\alpha_1} + \frac{\rho_2 c_2^2}{\alpha_2}\right) \frac{D\alpha_1}{Dt} - (\rho_2 c_2^2 - \rho_1 c_1^2)\nabla \cdot \mathbf{u}\right) \tag{25b}$$

Then using the volume fraction equation (17a) in (25) we get

$$\alpha_1 \rho_1 T_1 \frac{Ds_1}{Dt} = \left(1 - \frac{p}{\Phi}\right) \theta (T_2 - T_1) \tag{26a}$$

$$\alpha_2 \rho_2 T_2 \frac{Ds_2}{Dt} = -\left(1 - \frac{p}{\Phi}\right) \theta (T_2 - T_1) \tag{26b}$$

Combining these equations we get the following equation for the mixture entropy

$$\frac{\partial \rho s}{\partial t} + \nabla \cdot (\rho s \mathbf{u}) = \theta \left(1 - \frac{p}{\Phi}\right) \frac{(T_2 - T_1)^2}{T_1 T_2} \tag{27}$$

where $\rho s = \alpha_1 \rho_1 s_1 + \alpha_2 \rho_2 s_2$

According to the second law of thermodynamics

$$\frac{\partial \rho s}{\partial t} + \nabla \cdot (\rho s \mathbf{u}) = \theta \left(1 - \frac{p}{\Phi}\right) \frac{(T_2 - T_1)^2}{T_1 T_2} \geq 0 \tag{28}$$

Thus we want that

$$\Phi \geq p \tag{29}$$

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Numerical Results

- Initially we consider the radius of the bubble $R_{max} = 0.75\ mm$.
- The pressure inside the bubble equals to the saturated vapor pressure $p_{sat} = 2330\ pa$.
- The pressure of the water is $1\ bar$.
- The temperature inside and outside the bubble is $293.15\ K$.
- The interval of computations is $[0, 20R_{max}]$ in radial direction.

We compare our results with the experimental results of [6].

[6] S. Müller, M. Bachmann, D. Kröninger, Th. Kurz and Ph. Helluy, Comparison and Validation of Compressible Flow Simulations of Laser-Induced Cavitation Bubbles, Report No. 285, IGPM, RWTH Aachen, 2008.

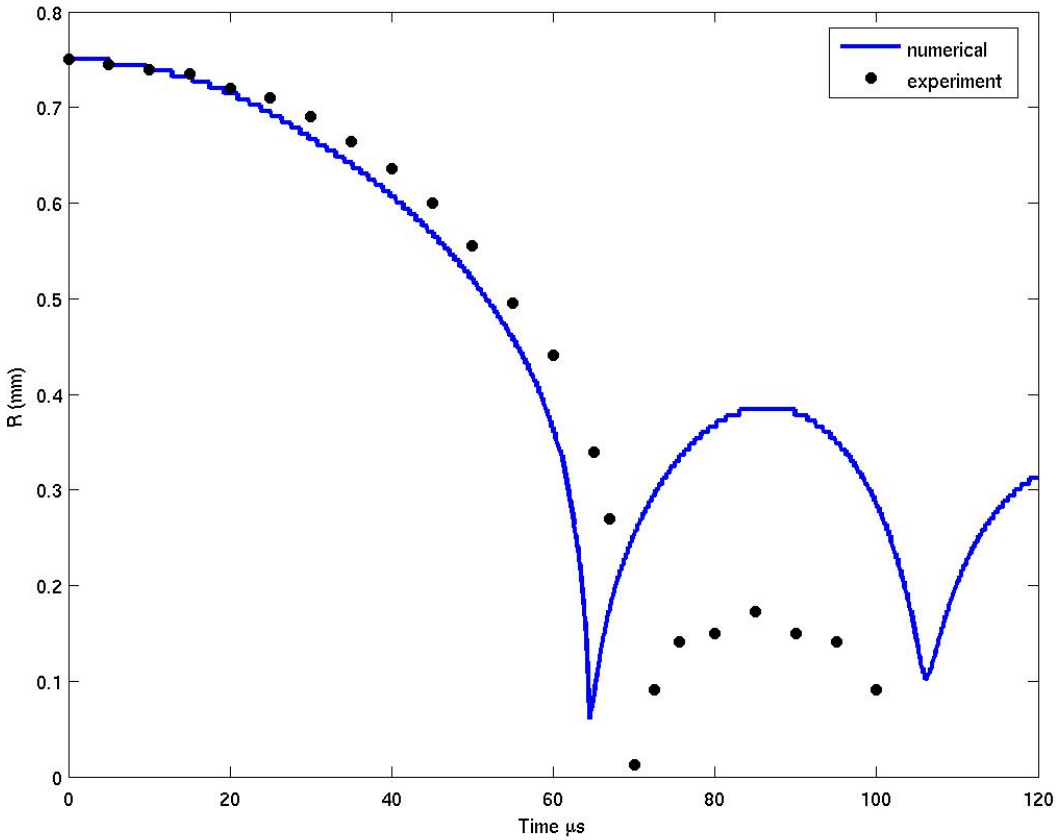

Figure 1: The collapse and the rebound of the radius of the bubble versus time, HLLC 2500 cells

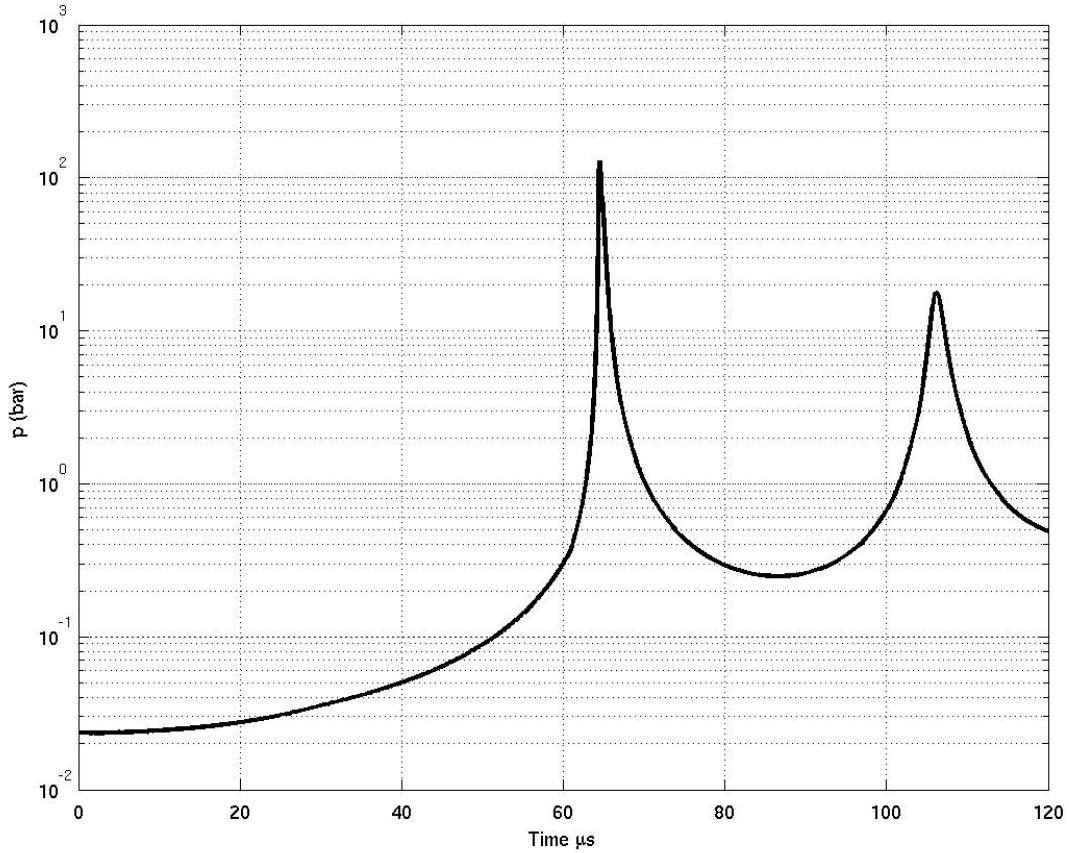

Figure 2: The pressure at the center of the bubble versus time, HLLC 2500 cells

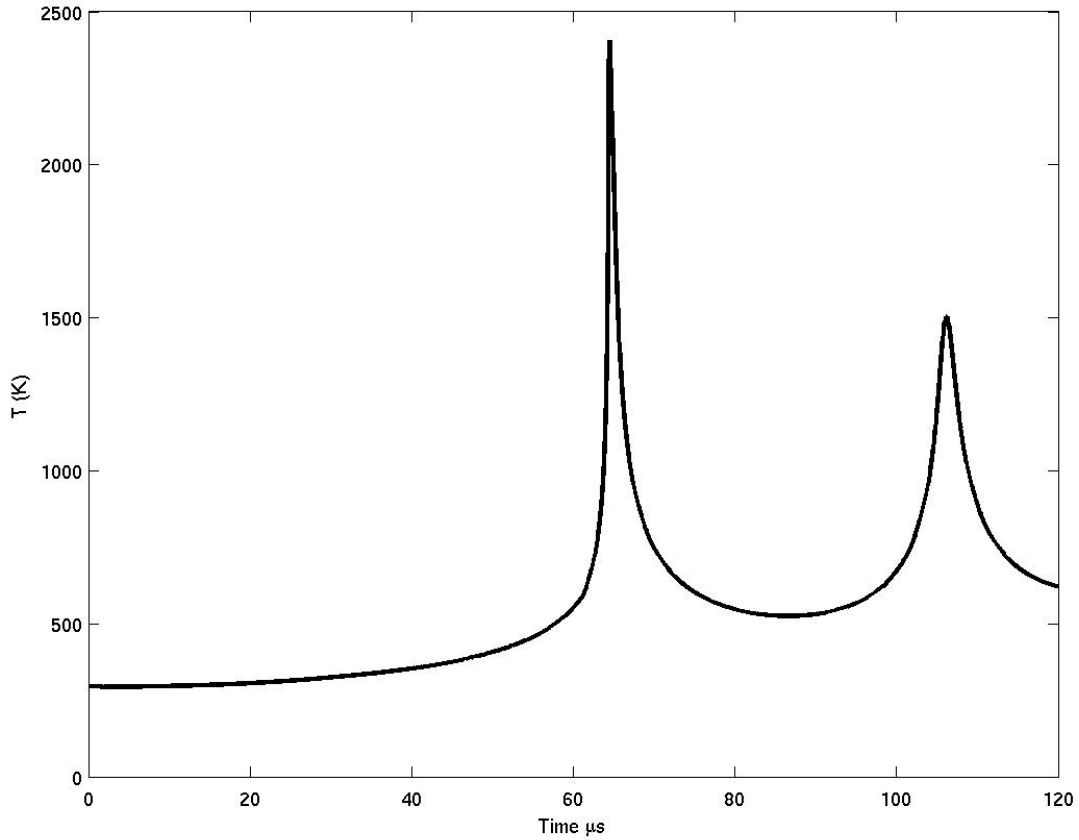

Figure 3: The temperature at the center of the bubble versus time, HLLC 2500 cells

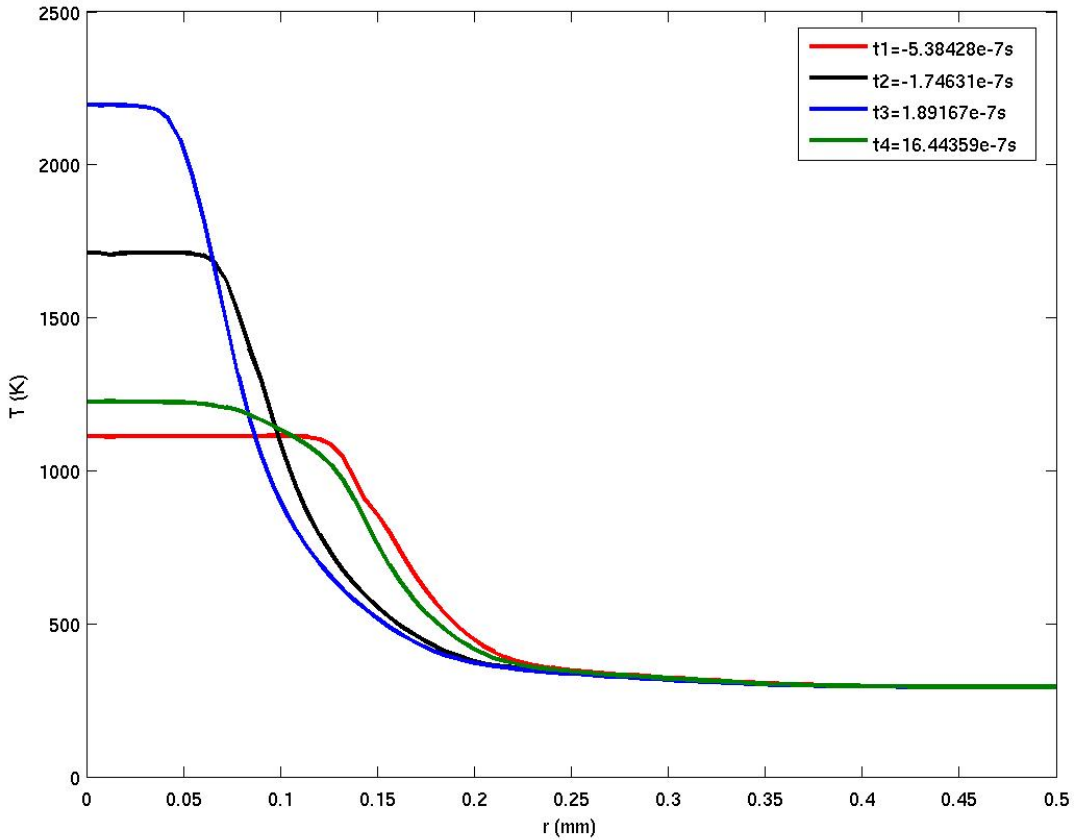

Figure 4: Spatial profiles of temperature at four moments of time, time is shown with respect to the collapse moment, HLLC 2500 cells

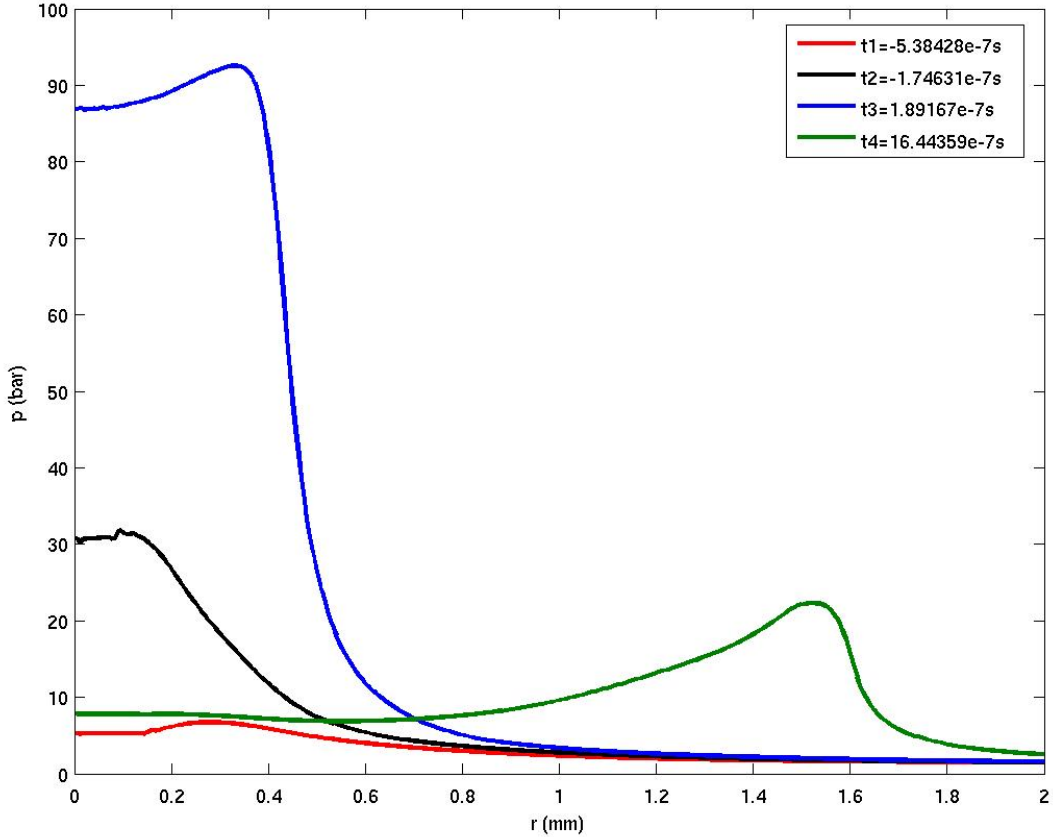

Figure 5: Spatial profiles of pressure at four moments of time, time is shown with respect to the collapse moment, HLLC 2500 cells

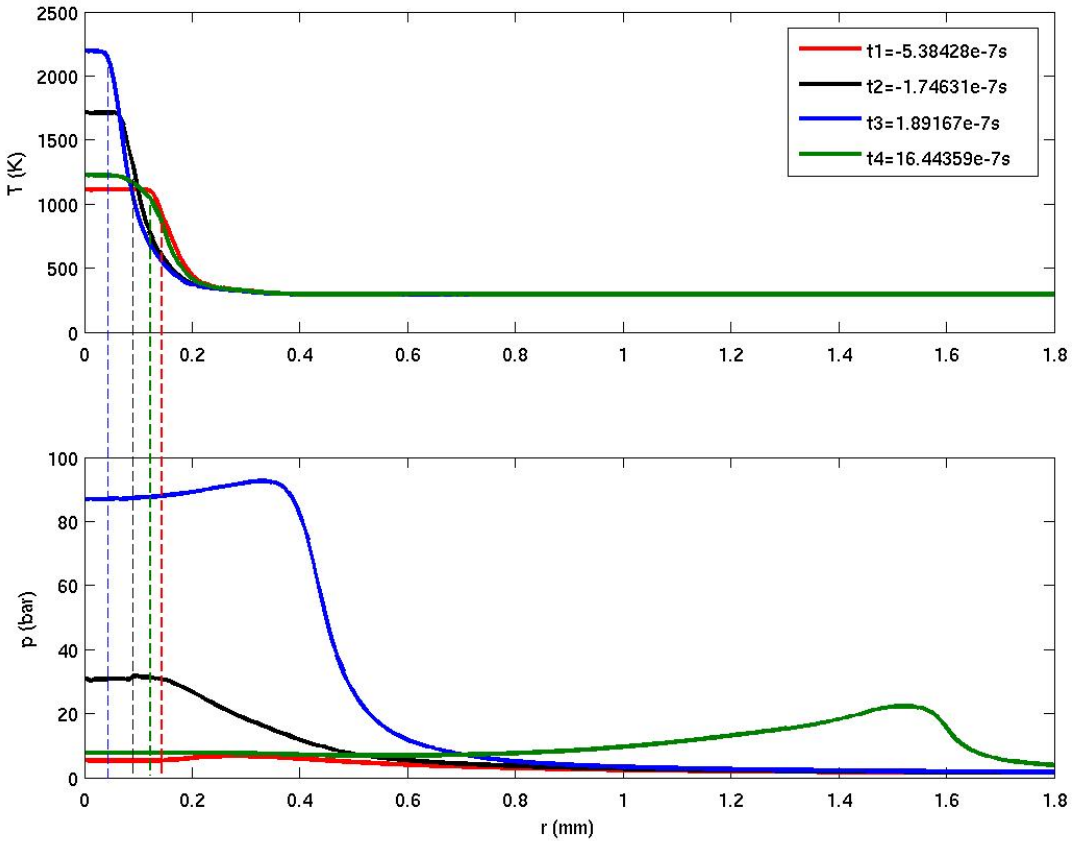

Figure 6: Spatial profiles of pressure and temperature at four moments of time, time is shown with respect to the collapse moment, vertical lines mark the vapor bubble radius, HLLC 2500 cells

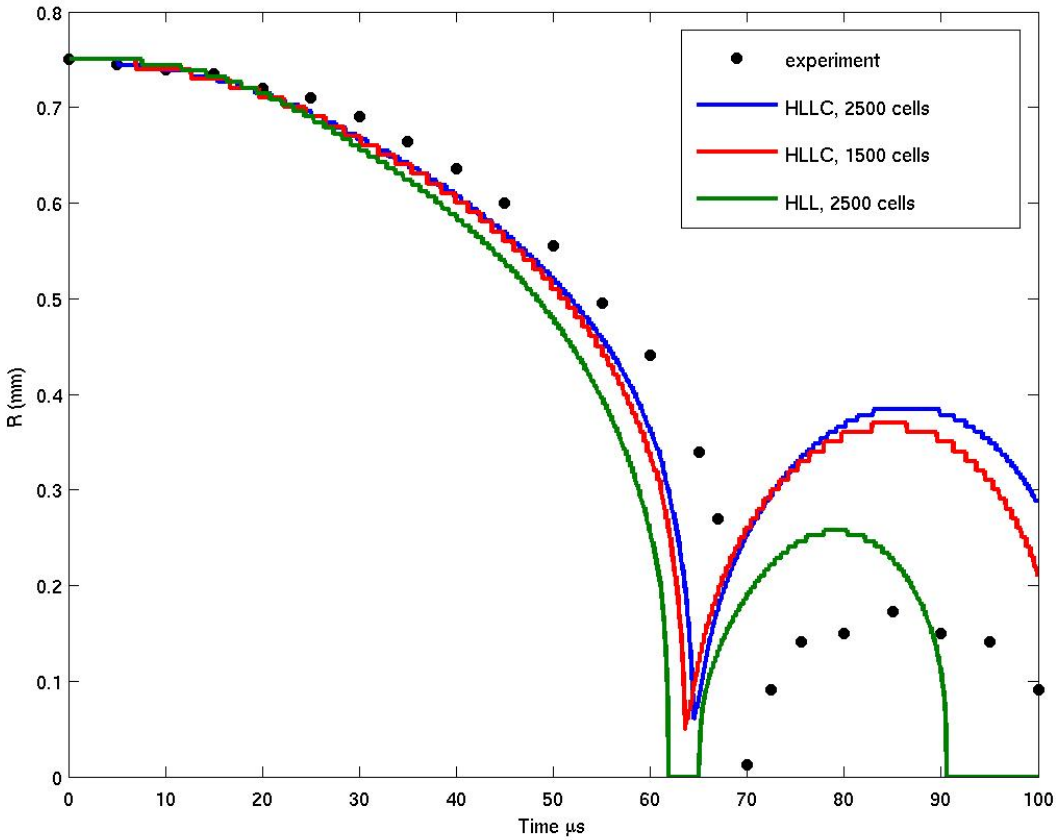

Figure 7: The collapse and the rebound of the radius of the bubble versus time, comparison

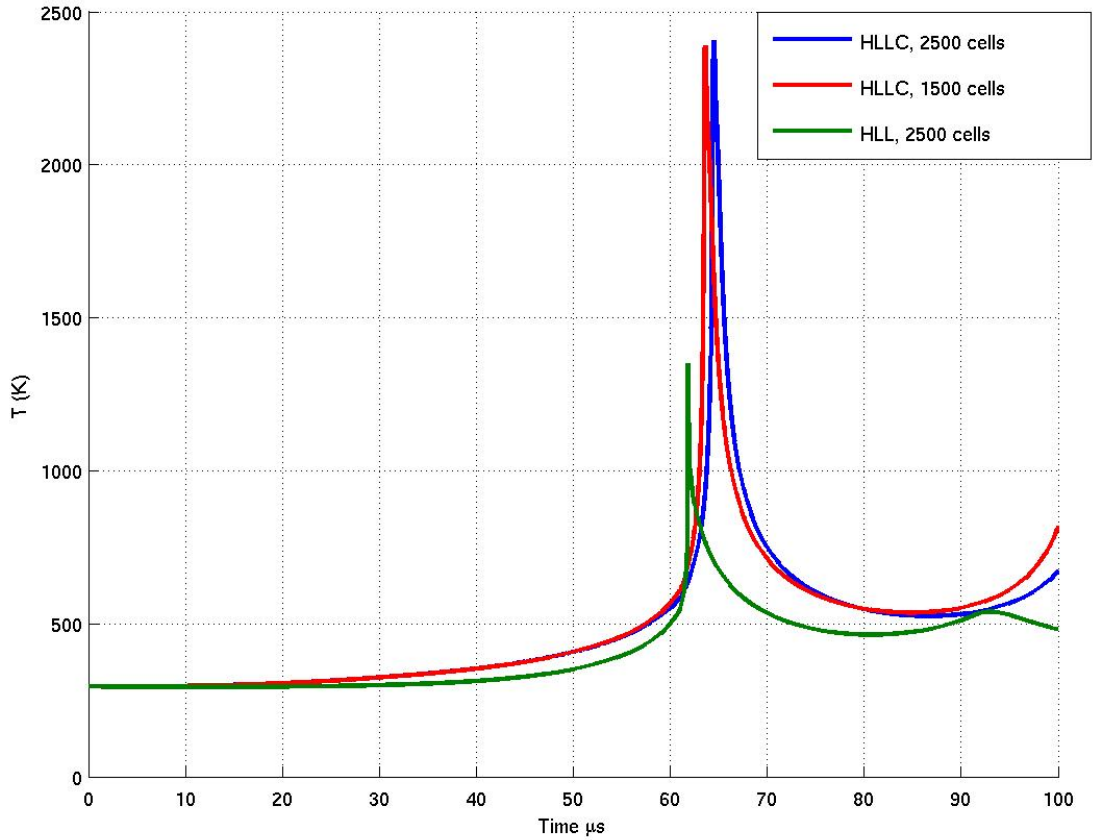

Figure 8: The temperature at the center of the bubble versus time, comparison

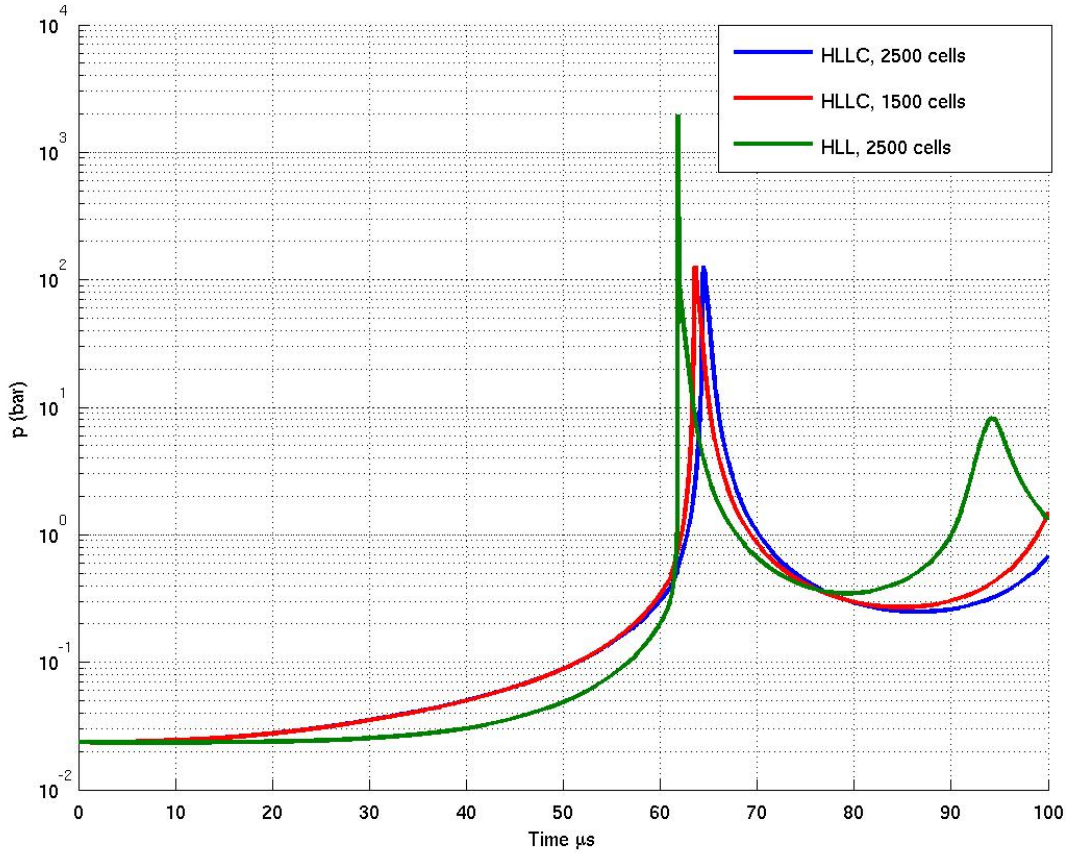

Figure 9: The pressure at the center of the bubble versus time, comparison

Outline

1. Introduction
2. Mathematical Model
3. Mathematical Properties of the Model
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Future Work

- Considering the phase transition
- Considering other Riemann solvers, i.e VFRoe
- Dealing with reduced models for one velocity, one pressure and/or one temperature.

References

[1] R. Saurel , R. Abgrall, A multiphase Godunov method for compressbile multifluid and multiphase flows, Journal of Computational Physics, 150 (2), 425-467, (1999).

[2] H. Guillard and M. Labois, Numerical modelling of compressible two-phase flows, European Conference on Computational Fluid Dynamics ECCOMAS CFD 2006, P. Wesseling and E. Onate and J. Priaux (Eds), 2006.

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