A level-set based free-surface tracking method for the simulation of bubble collapse and jetting in generalized Newtonian fluids

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Abstract

Predictive simulations of aspherical bubble collapse and jetting are known to be particularly challenging. Under the influence of an external pressure perturbation, bubbles can also undergo prolonged oscillations with potentially large variations in their size and shape. Simulation techniques must robustly represent these large variations while maintaining accuracy. The challenge of nonlinear rheology introduces additional challenges. To do this, we design a new level-set-based free-surface tracking technique. The bubble contents are assumed to be inviscid and spatially homogeneous, governed by a polytropic gas equation of state. A least-squares methodology enforces the normal pressure jump and shear-free boundary conditions precisely at the sharp bubble-liquid interface. Constraints maintain a divergence-free velocity. Numerical tests on spherically symmetric configurations on rectangular meshes demonstrate that the method accurately predicts the bubble response to impulsive and time-periodic pressure perturbations in a generalized Newtonian fluid over multiple growth and collapse cycles. Asymmetries remain small throughout the course of computations. Demonstrations of aspherical bubble dynamics and jetting next to a rigid wall illustrate the formulation's ability to represent complex topological features, including interface breakup in shear-thinning/thickening fluids. These simulations are used to study the influence of shear-thinning and shear-thickening rheology on cavitation damage in tissue-mimicking soft materials. Simulations of growth and collapse of a spherically symmetric vapor bubble that fully incorporate the phase change dynamics, illustrate the flexibility and robustness of our implementation.

Keywords: cavitation; bubble collapse; sharp interface method

Introduction

Cavitation bubble collapse plays an important role in a variety of biomedical techniques that involve interaction of shock or acoustic waves with tissue or blood [1-3]. In applications such as shock-wave and burst-wave lithotripsy, cavitation bubble collapse is thought to be principally responsible for both kidney stone comminution and undesirable collateral damage caused to the surrounding tissue. Similarly, microcavitation induced by the interaction of the tensile portion of the blast waves with brain tissue has been proposed as a likely cause for blast-wave-induced traumatic brain injury. Detailed understanding of the aspherical bubble collapse and jetting process in tissue-mimicking soft materials can aid design of damage-resistant shields that mitigate or suppress microcavitation-induced tissue injury and can help optimize biomedical techniques such as lithotripsy.

The bubble collapse process is intense and rapid with the entire process, including the formation of high-speed jet, typically lasting for only tens of microseconds for micron sized bubbles [1]. The violence of the collapse and jetting process cause high local stresses and strain rates. The mechanical properties of tissues differ vastly from those of simple fluids and under these extreme conditions the nonlinear rheology of the tissue material is expected to play an important role in the collapse, jetting, and injury [3]. The influence of complex rheology on the collapse and jetting dynamics is thus of significance and motivates our simulation-based analysis of aspherical bubble dynamics in shear-thinning and shear-thickening generalized Newtonian fluids.

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The nonlinearity in the constitutive relationship presents additional computational challenges in simulations of bubble growth and collapse in a rheologically complex fluid medium. To accurately account for the nonlinear rheology of a generalized Newtonian fluid medium, simulation methods are most faithful to the mechanics they represent if they ensure exact continuity of the normal and tangential stresses across the bubble surface. Enforcing this condition is particularly challenging in the commonly employed fully compressible formulations that integrate shock and interface capturing methodologies with techniques that ensure correct transmission of the shock and acoustic waves across the bubble-liquid interface [4-11]. Resolution of rheology-dependent sharp flow features, such as boundary layers, within a fully compressible formulation tends to be prohibitively expensive. This is due to the restrictions on spatiotemporal resolutions that must overcome the numerical dissipation fundamental to effective shock and interface capturing techniques. Important for motivating our formulation, for many relevant physiological conditions, the acoustic perturbations are relatively weak so that a general compressible treatment of the nearly incompressible liquid phase is overly descriptive, inefficient, and potentially inaccurate. To overcome the aforementioned challenges and limitations of a compressible multifluid treatment we develop a level-set-based free-surface tracking technique that fully incorporates the important complex rheology of the generalized Newtonian fluid medium but with approximations suited to our condition. In the subsequent sections, we describe our modeling and simulation approach, and demonstrate simulations of a near-wall bubble pair collapse in a shear-thinning fluid and a spherically symmetric collapse with inclusion of mass transfer across the interface.

Free-surface model for bubble dynamics

Typical cavitation-induced tissue damage scenarios involve interactions of micron-sized bubbles with relatively weak acoustic perturbations with a wavelength significantly larger than the bubble size. The bubble density and viscosity are typically orders of magnitude lower than those of the surrounding fluid. In such situations, spatial variations of the state variables in the bubble interior are negligible compared to those in the surrounding medium, which itself is very nearly incompressible. We therefore consider a modeling framework in which the bubble contents are assumed to be inviscid and spatially homogeneous, as in the well-established Rayleigh-Plesset model for spherical bubble dynamics [12-16]. The spatially uniform bubble density ρ_B is related to its uniform pressure P_B via a polytropic gas equation of state of the form $P_B = P_{B0} (\rho_B/\rho_{B0})^\gamma$, where γ is the polytropic exponent and subscript '0' denotes initial bubble pressure and density. The complex rheology of the incompressible medium surrounding the bubble is accounted for through a generalized Newtonian fluid model for the shear-dependent viscosity. Thus, within this relatively simplified framework, the shear-free bubble-medium interface simply serves as a boundary for the incompressible fluid medium. The principle novelty of the numerical discretization is enforcement of the kinematic and dynamic conditions at the interface to ensure continuity of the tangential and normal stresses across the material interface.

Numerical discretization

The method is built on a standard second-order accurate spatial discretization of the incompressible Navier-Stokes equations for a generalized Newtonian fluid. We employ a fully staggered arrangement of the primitive variables, taking advantage of its well-understood advantageous properties. The bubble boundary is tracked with an efficient narrow-band level-set technique, which relies on high-order advection and frequent reinitialization of a signed distance function [17]. A least-squares extrapolation method enforces the normal pressure jump and shear-free boundary conditions at the sharp bubble-medium interface. To minimize conservation errors in the transport of the level-set function, constraints are built into the extrapolation procedure for computing a divergence-free velocity field. We employ a second-order accurate explicit Runge-Kutta projection method for time advancement of the flow field and the bubble-medium interface.

Demonstration simulations

As a first demonstration example, we simulate axisymmetric growth and collapse of a bubble pair in a shear thinning medium next to a solid wall. The initially equisized gas ($\gamma = 1.4$) bubbles are located at non-dimensional stand-off distances of 2.33 and 5.0 (with the initial bubble radius R_0 as the characteristic length scale) from a left solid bound-

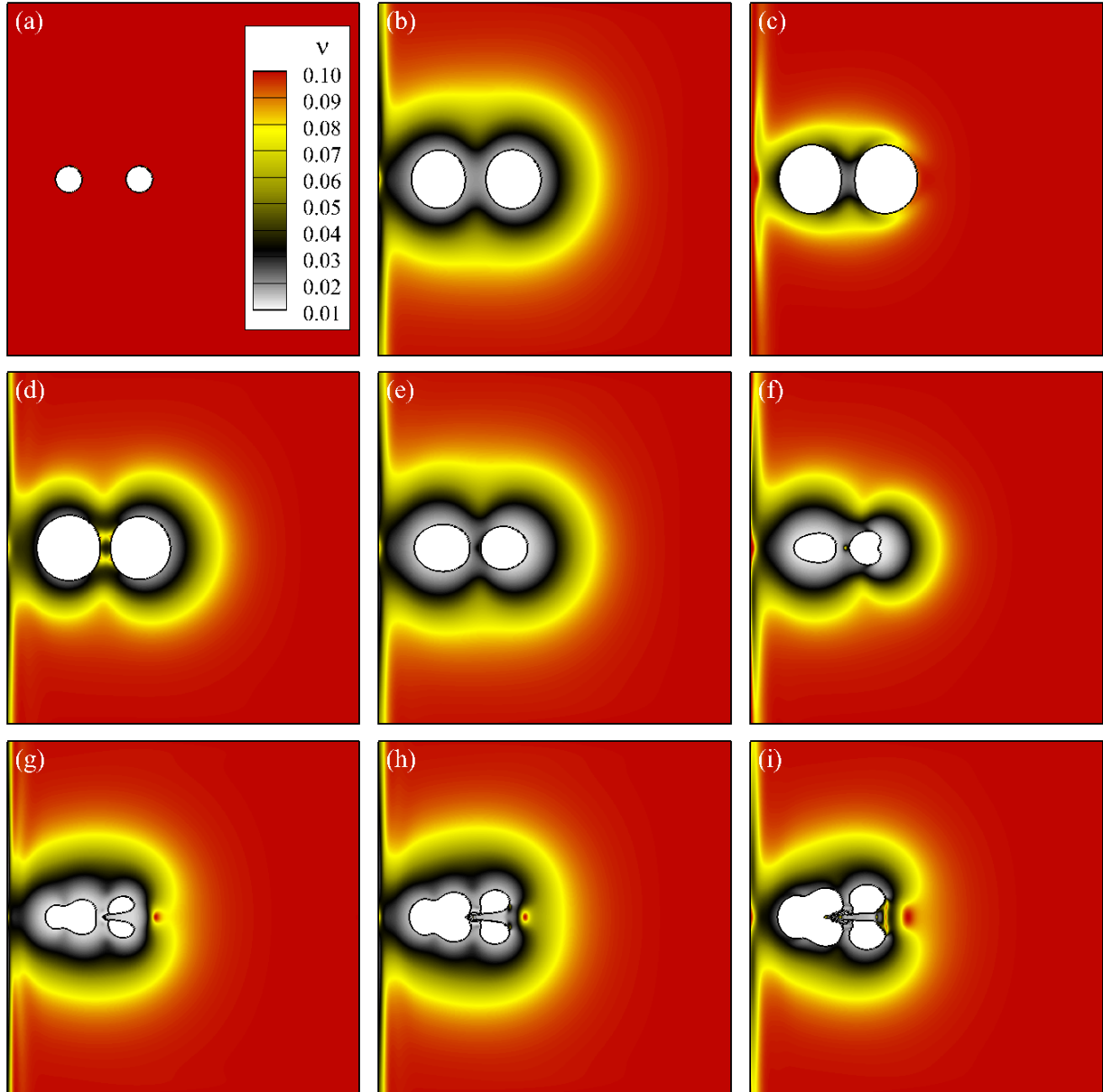*Corresponding Author, Ratnesh K. Shukla: ratnesh@iisc.ac.in

Figure 1: Generalized Newtonian viscosity (colors) and the shear-free bubble-liquid interface (solid black line) as a function of time for near-wall growth and collapse of a bubble pair in a shear-thinning fluid medium.

ary as depicted in figure 1(a). The initial bubble pressure P_{B0} is ten times the far-field pressure P_∞. No-slip and symmetry boundary conditions are applied at the left solid wall and lower boundary, while at the remaining two boundaries the far-field pressure P_∞ is prescribed along with a normal extrapolation for the velocity components. The shear-thinning is modeled with the commonly used Carreau expression [18]:

$$v(\dot{\gamma}) = v_\infty + \frac{v_0 - v_\infty}{\left(1 + \lambda^2 \dot{\gamma}^2\right)^{N/2}}$$

where limit viscosities are $v_0 = 0.1$ and $v_\infty = 0.01$, with the exponent $N = 0.8$. In this model, $\dot{\gamma}$ and λ denote the non-dimensional shear rate and a material constant, respectively.

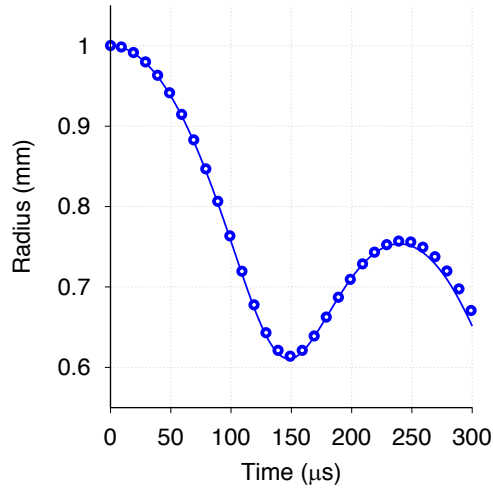*Corresponding Author, Ratnesh K. Shukla: ratnesh@iisc.ac.in

Figure 2: Radius histories of a spherically-symmetric vapor bubble collapse under an initial pressure ratio of 2 obtained from semi-analytical solution (line) and detailed axisymmetric simulation (symbols).

Figure 1 shows the evolution of the bubble-medium interface and the generalized Newtonian viscosity for a typical simulation on a uniform mesh with a spatial resolution that corresponds to about 19 nodes across the initial bubble radius R_0. The initial expansion of the bubble pair induces a shear-driven reduction in the generalized Newtonian viscosity around the bubble and in the boundary layer on the solid boundary. The reduction in the local viscosity, owing to an aspherical expansion of the two bubbles, eventually results in a jet formation and jetting impact (spherical to toroidal shape transition) of the bubble that is located further away from the solid boundary. However, this shear-thinning-induced local reduction in viscosity is less pronounced in the vicinity of the solid wall and therefore jet formation and therefore jetting impact is completely suppressed for the bubble located next to the solid boundary.

In our second example, we demonstrate the flexibility of our method to include phase change phenomenon. As a first step, we implemented a simplified from of the Hertz-Knudsen-Langmuir expression (see Hauke *et al.* [19] for details) for non-equilibrium mass transfer across the interface. The primary simplification we made here is that the saturation pressure in the mass transfer expression is assumed to be constant throughout the simulation, equal to the initial bubble pressure. For demonstration, we simulated spherically symmetric collapse of a vapor ($\gamma = 1.3$) bubble under an initial pressure ratio of 2. The bubble is assumed to be filled with saturated vapor initially at 50 kPa pressure; the mass transfer accommodation coefficient is set to 0.01. Figure 2 shows excellent agreement between the radius histories obtained from our axisymmetric simulation and the semi-analytical solution of a generalized Rayleigh-Plesset equation.

Summary

In summary, a sharp-interface Eulerian method that employs least-squares extrapolation in simulations of growth and collapse of multiple bubbles in an incompressible, generalized Newtonian fluid was presented. Axisymmetric simulations of near-wall growth and collapse of a bubble pair in a shear-thinning surrounding medium were conducted to demonstrate the method. In the examples considered, shear-thinning promotes jetting in aspherical bubble collapse through a reduction in the local generalized Newtonian viscosity. We also demonstrated the ability of our method to handle phase transition.

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