Bubble collapse near a fluid-fluid interface using the spectral element marker particle method with applications in bioengineering

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A B S T R A C T

The spectral element marker particle (SEMP) method is a high-order numerical scheme for modelling multiphase flow where the governing equations are discretised using the spectral element method and the (compressible) fluid phases are tracked using marker particles. Thus far, the method has been successfully applied to two-phase problems involving the collapse of a two-dimensional bubble in the vicinity of a rigid wall. In this article, the SEMP method is extended to include a third fluid phase before being applied to bubble collapse problems near a fluid-fluid interface. Two-phase bubble collapse near a rigid boundary (where a highly viscous third phase approximates the rigid boundary) is considered as validation of the method. A range of fluid parameter values and geometric configurations are studied before a bioengineering application is considered. A simplified model of (micro)bubble-cell interaction is presented, with the aim of gaining initial insights into the flow mechanisms behind sonoporation and microbubble-enhanced targeted drug delivery. Results from this model indicate that the non-local cell membrane distortion (blebbing) phenomenon often observed experimentally may result from stress propagation along the cell surface and so be hydrodynamical in origin.

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1. Introduction

The dynamics of bubble collapse has received substantial attention in the literature over the past 100 years. Starting with Lord Rayleigh (1917), who considered the collapse of a spherical cavity in an infinite expanse of incompressible fluid, subsequent experimental, numerical and analytical studies have highlighted a complex physical process, where possible observed phenomena include jet formation, pressure shockwave emission and toroidal bubble formation (see, for example, Benjamin and Ellis, 1966; Lauterborn and Ohl, 1997). Research is motivated by the prevalence of bubbles in nature and industry and their fundamental role in many fluid systems. Cavitation damage due to bubble collapse is now a well-known phenomenon, and has negative consequences in a number of areas. In biomedicine, for example, ultrasound mediated drug delivery (Hernot and Klibanov, 2008; Lentacker et al., 2014; Wu and Nyborg, 2008) and shock-wave lithotripsy procedures (Freund et al., 2009; Kodama and Takayama, 1998) can generate cavitation bubbles that may cause cell death and hemorrhaging in the surrounding tissue, respectively. However, bubbles may also be used to dissolve blood clots (see e.g. Unger et al., 2002), break through the blood-brain barrier (see e.g. Ting et al., 2012) and clean and sterilise surfaces (see e.g. Chahine et al., 2016; Song et al., 2004). Numerical studies of bubble dynamics have been dominated by the boundary element method (BEM), originally used in this context by Blake et al. (1986, 1987). The method requires the assumption of irrotationality, which considerably simplifies the governing equations. While this assumption has proven effective for moderate to high Reynolds numbers (Curtiss et al., 2013; Klaseboer and Kho, 2004a, b) and in cases of weak flow compressibility (Wang, 2014; Wang and Blake, 2010), it precludes some key physics necessary in the modelling of multiphase biomedical flows, such as strong compressibility (i.e. ultrasound) and general non-Newtonian effects.

Numerical solutions of the full Navier-Stokes equations for bubble dynamics problems have received considerably less attention in the literature than boundary elements, most likely due to the increased implementation difficulty and computational time. Shopov and Minev (1992); Shopov et al. (1990) and Shopov et al. (1992) considered a finite element approximation of the incompressible Navier-Stokes equations, where the mesh was fitted to the bubble surface and evolved in a Lagrangian manner. Fitting the computational mesh to the bubble surface could substantially increase the computational time, particularly under significant topological changes. Popinet and Zaleski (2002) produced a well-defined (unfitted) interface over a finite volume grid by
interpolating through bubble surface marker points using cubic splines. They found good agreement with experimental results for the incompressible phase of the dynamics but concluded that compressibility and thermal effects may be required for the compressible phase (bubble rebound).

Wang and Blake (2010) developed an approximate theory for bubble dynamics in a compressible fluid using matched asymptotic expansions. The perturbation was performed to second order using the bubble-wall Mach number (assumed to be small). The bubble dynamics could then be numerically modelled using traditional boundary elements with compressibility appearing in the far-field boundary condition. Due to the assumption of a small Mach number, the method may not be able to accurately capture the bubble behaviour during the latter stages of collapse when larger degrees of compressibility may be required. However, excellent agreement was found with the Keller-Herring equation for spherical bubbles and test cases included the behaviour of a bubble under both a weak and strong acoustic wave. Wang (2014) subsequently applied the compressible BEM model to bubble collapse near a rigid wall. During the incompressible phase of the bubble dynamics, Wang (2014) achieved excellent agreement with experimental observations. During the bubble rebound, where compressibility is important, the agreement was an improvement on previous results (e.g. Popinet and Zaleski, 2002) but still differed when compared to experiments (see their Fig. 7). It is likely that the secondary collapse phase required an amount of compressibility which is beyond the scope of the BEM model. In their boundary element study, (Lee et al., 2007) took a different approach and approximated compressible effects by incorporating a loss in energy (provided by experimental data) during the bubble rebound and found very good agreement with experimental results, including the capture of the elusive counterjet. Müller et al. (2010) considered collapse of a gas filled bubble near a rigid wall using a finite volume technique for the compressible Euler equations. They showed that when a bubble collapses near a rigid wall (in the absence of viscosity, buoyancy and surface tension), the compressible bubble contents interact with reflected pressure shock-waves (caused by the oscillation of the bubble), producing vortices in the gaseous bubble contents. These vortices rotate in opposite directions and are directed towards the rigid wall. The vortices pull the gaseous bubble contents and bubble surface towards the rigid wall producing the well-known toroidal shape and high-speed liquid jet. Importantly, these are observations which cannot be obtained from incompressible and irrotational simulations such as BEM. The above studies, particularly that of Müller et al. (2010), illustrate the importance of compressibility, even in situations commonly assumed to be predominantly incompressible. It is evident that if compressible effects are to be included then the full compressible Navier-Stokes (or Euler) equations must be considered.

Lind and Phillips developed a Spectral Element Marker Particle (SEMP) method for fully compressible bubble collapse problems in both Newtonian (Lind and Phillips, 2012) and viscoelastic fluids (Lind and Phillips, 2013) with small to moderate Reynolds numbers. SEMP uses the marker particle method (Rider and Kothe, 1995) to track the fluid phases. The marker particle method is Lagrangian in nature and bears semblance to both the VOF (Hirt and Nichols, 1981) and the MAC (Harlow and Welch, 1965) methods. A colour function C is determined by tracking massless marker particles. Each particle is assigned a particular colour depending upon the phase in which it resides, and because a particle of fluid will remain of that fluid type (assuming no change in phase), a particle will keep its colour indefinitely. Within fluid-fluid interface regions, where two (or more) differently coloured sets of marker particles reside, a weighted average is taken of the surrounding particles to determine an interpolated colour at a desired grid point. In this article, SEMP is extended to include a third phase, that may be used to model deformable biological matter (e.g. cells or tissue). While there have been a number of works considering bubble collapse near deformable surfaces (see e.g. Klaseboer and Khoo, 2004b; Ohl et al., 2009), few include sufficient physics to model the complex multiphase biomedical processes that motivate this work. Indeed, the eventual aim is to gain insights into the flow mechanisms behind sonoporation (e.g. Lentacker et al., 2014) and microbubble-enhanced targeted drug delivery (e.g. Hernot and Klibanov, 2008).

This article is structured as follows. The mathematical model and governing equations are introduced in Section 2 with their numerical approximation discussed in Section 3. The three-phase method is validated in Section 4 before a numerical investigation into the effect of viscosity and the thickness of the third phase is given in Section 5. A simplified model of (micro)bubble-cell interaction is presented in Section 6 before the article is concluded in Section 7.

2. The mathematical model and governing equations

Consider a two-dimensional (2D) domain Ω, which contains a gas-filled bubble Ω_b of initial density ρ_b, surrounded by fluid Ω_f of initial density ρ_f, placed near a fluid layer Ω_r such that Ω_r = Ω \ (Ω_f ∪ Ω_b). Note that all variables with index b will refer to those associated with the bubble, those labelled f with the ambient fluid and those labelled c with the fluid layer. A schematic is given in Fig. 1.

In general, the equations governing fluid motion are the mathematical statements of conservation of momentum

$$\rho \frac{Du}{Dt} = -\nabla p + \nabla \cdot \mathbf{S}, \quad (1)$$

and conservation of mass

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{u} = 0,$$

where \(\mathbf{u}\) is the velocity, \(\mathbf{S}\) is the extra-stress tensor and \(\rho\) is the density. In the majority of bubble simulations in the literature (see e.g. Blake et al., 1986; Curtiss et al., 2013; Lee et al., 2007; Popinet and Zaleski, 2002), the fluid phases are assumed to be incompressible. However, in modelling bubble dynamics, particularly growth or collapse, one needs to account for the change in volume of the bubble, and so any fluid that may reside within must be modelled as compressible. Furthermore, and as discussed in the introduction, compressibility is known to play an important role in the final stages of bubble collapse, contributing significantly to energy dissipation (Lee et al., 2007). Also, in the context of biomedical flows, if one requires accurate descriptions of any acoustic fields applied to or emitted from the bubble, compressibility and the complete conservation of mass equation must be retained. Accordingly, a thermodynamic equation of
state is required to close the system of governing equations. Following Lind and Phillips (2012), the equation of state is taken to be the ideal gas law, namely

$$p = \frac{c^2}{\gamma} \rho = \rho \bar{c}^2.$$  \hspace{1cm} (2)

where $c$ is the speed of sound within the medium, $\gamma$ is the ratio of specific heats (adiabatic index) and $\bar{c} = c/\sqrt{\gamma}$. The specific heat ratio typically takes values between 1 and 1.7, for a range of different gases of various molecular weights and temperatures (White, 2010). The value of $\sqrt{\gamma}$ is, therefore, close to one, and so we take $\bar{c} = c$ throughout this paper as a first approximation. Despite its simplicity (and limitations), (2) is a useful model (Lind and Phillips, 2012; 2013). Firstly, it provides a reasonably accurate thermodynamic description of the bubbles gaseous contents. Secondly, by variation of a single model parameter one can easily explore the effect of compressibility on the flow, and readily recover near-incompressibility, if required.

The constitutive equation, or rheological equation of state, for a compressible Newtonian fluid is well known. The extra-stress tensor is given by

$$\mathbf{S} = \eta_1 (\nabla \mathbf{u} + \nabla \mathbf{u}^T) + \eta_2 (\nabla \cdot \mathbf{u}) \mathbf{I},$$  \hspace{1cm} (3)

where $\nabla \mathbf{u}$ is the velocity gradient, the superscript $T$ denotes the transpose, $\mathbf{I}$ is the identity tensor and $\eta_{1,2}$ are scalar coefficients. Commonly, $\eta_1$ is named the (dynamic) shear viscosity coefficient and $\eta_2$ is termed the dilatational viscosity coefficient. Eq. (3) is the most general constitutive equation for a Newtonian fluid as it imposes no restrictions on compressibility or on $\eta_{1,2}$. Often one abides by Stokes hypothesis and sets the bulk viscosity $\kappa = (\frac{1}{2} \eta_1 + \eta_2)$ to zero (Gad-el-Hak, 1995). As stated in Lind and Phillips (2012), this implies that the mean mechanical pressure $p^*$ becomes equivalent to the thermodynamic pressure $p$ in Eq. (1) and that the extra stress is trace free: $\sum_i S_{ii} = 0$. However, in this work Stokes’ hypothesis is not adopted and the most general form of the compressible Newtonian extra-stress tensor (Eq. (3)) is retained.

2.1. Nondimensionalisation of the governing equations

This article employs a similar non-dimensionalisation as used in Lind and Phillips (2012): distances are scaled with respect to initial bubble radius $R$, densities are scaled with respect to the initial bubble density $\rho_{0,b}$, pressures are scaled with respect to $\rho_{0,b} V^2$, where $V$ is a reference speed of sound (e.g. the speed of sound through an ideal gas), and stresses are scaled with respect to $\rho_{0,b} V^2$. Consequently, the non-dimensional viscosities $\eta^*$ are scaled according to

$$\eta^* = \frac{\eta}{\rho_{0,b} V^2}.$$  

A Reynolds number can be defined as $Re = 1/\eta^*$, but it is more beneficial to refer to non-dimensional viscosities due to the several viscous parameters present in compressible models. Therefore, dropping the asterisks and substituting Eq. (2) into Eq. (1), the non-dimensional governing equations for a compressible Newtonian fluid are: the conservation of momentum

$$\frac{Dp}{Dt} = -c^2 \nabla \rho + \nabla \cdot \mathbf{S},$$  \hspace{1cm} (4)

the conservation of mass

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{u} = 0,$$  \hspace{1cm} (5)

and the constitutive equation

$$\mathbf{S} = \eta_1 (\nabla \mathbf{u} + \nabla \mathbf{u}^T) + \eta_2 (\nabla \cdot \mathbf{u}) \mathbf{I}. $$  \hspace{1cm} (6)

As in Lind and Phillips (2012), a log-density formulation is implemented where the governing equations are solved for log density $q := \ln(\rho)$ and a kinematic stress $\mathbf{S} := \rho \mathbf{T}$. The standard and log-density formulations of the governing equations are physically equivalent, but the log-density formulation is convenient as the coupled mass and momentum equations become predominantly linear for constant kinematic viscosity (Bollada and Phillips, 2007; 2008). There are also numerical stability benefits for multiphase flows as potentially large density differences across interfaces are scaled down in magnitude when working with the log density. Accordingly, any subsequent reference to the density or stress will technically refer to the log density and kinematic stress, as defined above.

3. Numerical solution of the governing equations

3.1. Time discretisation

In this article, a semi-Lagrangian approximation of the material derivative is used for both the conservation of momentum and mass equations (Eqs. (4) and (5)), (Bollada and Phillips, 2007, 2008). A notable feature of the semi-Lagrangian scheme is that it can relieve the time step (CFL) restriction. When the semi-Lagrangian scheme is used in conjunction with the spectral element method (as is the case here), the restriction on the size of the time-step is due to accuracy considerations rather than stability (Karniadakis and Sherwin, 2005). Such accuracy considerations can be informed by the work of Falcone and Ferretti (1998), where it is shown (for the one-dimensional advection-diffusion equation with a finite element type method) that the overall error of semi-Lagrangian schemes is given by

$$O\left(\Delta t^2 + \frac{\Delta x^{N+1}}{\Delta t}\right),$$  \hspace{1cm} (7)

where $N$ is the polynomial degree of the spatial approximation and $K$ is the order of the backward integration step. In this article, we employ a first-order Lagrangian approximation of the material derivative:

$$\frac{D\mathbf{u}}{Dt} = \frac{\mathbf{u}^{n+1}(\mathbf{x}^n) - \mathbf{u}^{n}(\mathbf{x}^n)}{\Delta t} = f(\mathbf{u}^{n+1}),$$  \hspace{1cm} (8)

where $\mathbf{u}^n(\mathbf{x}) = \mathbf{u}(\mathbf{x}, t^n)$ is the velocity of a fluid particle $\mathbf{x}$ at time $t^n = n \Delta t$, $n = 1, \ldots, N_t$ (where $N_t$ is the total number of time steps), $\mathbf{x}^n = \mathbf{x}(t^n)$ denotes the position of a fluid particle at time $t^n$ and $f$ is the right hand side of the momentum equation. Given $\mathbf{u}^n$, we wish to solve Eq. (8) implicitly for $\mathbf{u}^{n+1}$ for each nodal point. Hence, in order to approximate the material derivative, the previous position $\mathbf{x}^n$ of the fluid particle that moves onto the nodal point $\mathbf{x}^{n+1}$ is required, in addition to the velocity $\mathbf{u}^{n+1}$. In this article, we employ a second-order mid-point rule to determine the previous position $\mathbf{x}^n$, which is typical for semi-Lagrangian schemes (Karniadakis and Sherwin, 2005). The velocity $\mathbf{u}^{n+1}$ and position $\mathbf{x}^{n+1}$ are found iteratively and further details of the algorithm used can be found in Lind and Phillips (2012). Although the use of a higher-order semi-Lagrangian scheme is possible, it would require the calculation of at least two previous positions $\mathbf{x}^n$ and $\mathbf{x}^{n+1}$. As a high-order spatial approximation is employed in this article, it can be seen from Eq. (7), that the overall error in the scheme is dominated by the backward integration step (i.e. the calculation of the previous position). Thus, in calculating the multiple previous positions a compounding of the backward integration error could be seen. Although this error could be reduced by using a high-order backward integration step, it would increase the computational time for each step. Therefore, given the relatively small time-step $O(10^{-3})$ used in this article, we continue to employ the robust first-order scheme, successfully employed by Lind and Phillips (2012).
To summarise, the semi-discrete governing equations (in log-density formulation), which will shortly be discretised in space using the spectral element method, are given by: conservation of momentum
\[
\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} = -\mathbf{\nabla} q^{n+1} + \mathbf{T}^{n+1} + \nabla \cdot \mathbf{T}^{n+1},
\]
the conservation of mass
\[
\frac{q^{n+1} - q^n}{\Delta t} + \nabla \cdot \mathbf{u}^{n+1} = 0,
\]
and the constitutive equation
\[
\mathbf{T}^{n+1} = \mu_1 \left( \nabla \mathbf{u}^{n+1} + (\nabla \mathbf{u}^{n+1})^T \right) + \mu_2 (\nabla \cdot \mathbf{u}^{n+1}) \mathbf{I},
\]
where \( \mu_{1,2} = \eta_{1,2}/\rho \).

3.2. Spectral element method

The spectral element method (SEM) was first proposed by Patera (1984) to extend the application of spectral methods to problems defined in complex geometries. SEM has the geometric flexibility of a finite element method (FEM) with the accuracy of a spectral method and therefore, in principle is similar to hp - FEM. It is well-known that the SEM should perform better than traditional finite elements both in terms of accuracy and efficiency provided the solution is sufficiently regular and the accepted error level is sufficiently stringent (Patera, 1984).

3.2.1. Weak formulation

As stated at the beginning of this section, the whole domain \( \Omega \subset \mathbb{R}^2 \) contains the bubble \( \Omega_b \), the fluid layer \( \Omega_f \) and the ambient fluid \( \Omega_a \) such that \( \Omega_f = \Omega \setminus (\Omega_b \cup \Omega_a) \). The spectral element method is based on solving the governing equations in their equivalent weak form. Thus, the dependent variables \( \mathbf{u}, q \) and \( T \) are chosen from the following function spaces:
\[
\mathbf{u} \in \mathcal{V} := \left[ H^1(\Omega) \right]^2, \quad q \in \mathcal{Q} := H^1(\Omega), \quad T \in \mathcal{I} := \left[ H^1(\Omega) \right]^{2 \times 2},
\]
where \( H^1(\Omega) \) is a Sobolev space whose elements, and their first weak derivatives, are in \( L^2(\Omega) \) (Adams and Fournier, 2003). \( H^1(\Omega) \) contains any elements of \( H^1(\Omega) \) whose trace to the boundary \( \partial \Omega \) is zero and \( \left[ H^1(\Omega) \right]^{2 \times 2} \) contains all \( 2 \times 2 \), symmetric tensors whose components are elements of \( H^1(\Omega) \). Multiplying the strong form of the governing equations by an appropriate test function and integrating yields the following semi-discrete weak formulation: find \((\mathbf{u}, q, T) \) in \( \mathcal{V} \times \mathcal{Q} \times \mathcal{I} \) such that
\[
\int_\Omega \frac{\mathbf{u} - \mathbf{u}^n}{\Delta t} \cdot \mathbf{v} \, d\Omega + \int_\Omega \nabla q \cdot \mathbf{v} \, d\Omega = c^2 \int_\Omega \nabla \cdot \mathbf{v} \, d\Omega + \int_\Omega \nabla q \cdot \mathbf{T} \cdot \mathbf{v} \, d\Omega, \quad \forall \mathbf{v} \in \mathcal{V}, \quad (9a)
\]
\[
\int_\Omega \frac{q-q^n}{\Delta t} + \nabla \cdot \mathbf{u} \, d\Omega = 0, \quad \forall q \in \mathcal{Q}, \quad (9b)
\]
\[
\int_\Omega T : W \, d\Omega - \int_\Omega \mu_1 \nabla \cdot u : (W + W^T) \, d\Omega = \int_\Omega \mu_2 \nabla \cdot u \text{tr}(W) \, d\Omega, \quad \forall W \in \mathcal{I}, \quad (9c)
\]
where \text{tr}(W) is the trace of a tensor.

3.2.2. Spatial discretisation

In the spatial discretisation of the weak formulation (9) using the spectral element method, it is necessary to choose conforming discrete subspaces \( \mathcal{V}_h \subset \mathcal{V}, \mathcal{Q}_h \subset \mathcal{Q} \) and \( \mathcal{I}_h \subset \mathcal{I} \). The domain \( \Omega \) is divided into a number of non-overlapping, conforming, convex, quadrilateral spectral elements labelled \( \Omega_{\alpha,\beta} \). The coordinates \((\alpha, \beta)\) label each spectral element such that \( \alpha = 0, \ldots, 3 \) and \( \beta = 0, \ldots, \beta_{\text{max}} \). Thus, \( \alpha_{\text{max}} = (\alpha + 1) \) and \( \beta_{\text{max}} = (\beta + 1) \) denote the number of elements in the \( x \) and \( y \) directions respectively.

Let \( \mathcal{P}_N(\alpha,\beta) \) denote the space of all polynomials on \( \Omega_{\alpha,\beta} \) of degree less than or equal to \( N \) and define:
\[
\mathcal{P}_N(\Omega) := \left\{ \phi : \phi|_{\Omega_{\alpha,\beta}} \in \mathcal{P}_N(\alpha,\beta) \right\}
\]
The velocity, density and stress approximation spaces may then be defined as:
\[
\mathcal{V}_h := \mathcal{V} \cap \mathcal{P}_N(\Omega), \quad \mathcal{Q}_h := \mathcal{Q} \cap \mathcal{P}_N(\Omega), \quad \mathcal{T}_h := \mathcal{T} \cap \mathcal{P}_N(\Omega)^{2 \times 2},
\]
where it is understood that \( \mathcal{P}_N(\Omega)^{2 \times 2} \) defines each component of a tensor to be a member of \( \mathcal{P}_N(\Omega) \). Note that the density and velocity approximation space are both of degree \( N \). While compatibility conditions for the velocity and pressure (not density) approximation spaces are known for incompressible flow, we emphasize that no inf-sup stability issues have been seen in our compressible computations. Each spectral element is mapped to the parent domain \( D = [-1, 1] \times [-1, 1] \) using a transfinite mapping, \( F \), of Schneidersch and Deville (1992), where for each point \( \xi = (\xi, \zeta) \in D \) there exists a point \( \mathbf{x} = (x(\xi, \zeta), y(\xi, \zeta)) \in \Omega_{\alpha,\beta} \), such that \( x = F(\xi) \) and the vertices of \( \Omega_{\alpha,\beta} \) are given by \( x_1, \ldots, x_4 \). The velocity, density and stress are approximated on each element using Lagrangian interpolation through a select set of nodal points, called Gauss–Lobatto Legendre (GLL) points. In one dimension, the \( (N+1) \) GLL points are roots of the polynomial \( (1 - \xi^2)^N \) where \( N \) is the Legendre polynomial of degree \( N \). Therefore, the Lagrange interpolant can be shown to take the form
\[
h_i(\xi) = -\frac{(1 - \xi^2)^N}{N(N+1)} L_N(\xi),
\]
where \( \xi_i, i = 0, \ldots, N \) are the GLL points. The Legendre polynomials are a subset of polynomial eigenfunctions (Jacobi polynomials) of the singular Sturm–Liouville differential operator and it is well known, that the expansion of a C∞ function in terms of these eigenfunctions converges with spectral accuracy (exponential rates of convergence). Hence, an expansion in terms of the Lagrange interpolants (11) exhibits spectral properties, while also naturally lending itself to Gauss–Lobatto Legendre numerical quadrature. This is an improvement over traditional \( (h\text{-type}) \) finite element methods, which exhibit algebraic rates of convergence.

In 2D the GLL points form a \( (N+1)^2 \) grid within each element, interpolation over which yields the representation of each velocity component, stress component and density over the parent element
\[
u^\alpha(\xi, \zeta) = \sum_{i=0}^{N} \sum_{j=0}^{N} u^\alpha_{ij} h_i(\xi) h_j(\zeta),
\]
\[
T^{\alpha,\beta}(\xi, \zeta) = \sum_{i=0}^{N} \sum_{j=0}^{N} T^{\alpha,\beta}_{ij} h_i(\xi) h_j(\zeta),
\]
\[
q(\xi, \zeta) = \sum_{i=0}^{N} \sum_{j=0}^{N} q_{ij} h_i(\xi) h_j(\zeta),
\]
where \( u^\alpha_{ij}, T^{\alpha,\beta}_{ij} \) and \( q_{ij} \) are the approximations to \( u^\alpha, T^{\alpha,\beta} \) and \( q \) at each GLL point \( (\xi_i, \zeta_j) \), respectively. For more details regarding the spectral approximation, the reader is referred to the monograph of Karniadakis and Sherwin (2005).
where the weights \( w_i \) are chosen so that the quadrature rule is exact for polynomials of degree less than or equal to \( 2N - 1 \) (Owens and Phillips, 2002). The fully discrete equations are then obtained by inserting the variable expansions (Eq. (12)) into the weak form (Eq. (9)) and applying the above quadrature rule. For details of the full discrete system, the reader is referred to Lind and Phillips (2012).

### 3.3. The marker particle method

The marker particle method is a Lagrangian scheme to track multiple fluid phases and interfaces. A large number of markers placed within the domain act as markers, providing the identity of the fluid at a point in time and space. The approach was first suggested by Rider and Kothe (1995) and compares favourably with VOF and level set methods. Particular benefits include the absence of numerical mass diffusion and numerical surface tension, and the ability to handle severe topological changes with ease. Furthermore, the scheme is straightforward to implement and is very robust (Rider and Kothe, 1995). It has been subsequently applied in Newtonian drop dynamics studies by Bierbrauer and Zhu (2007) and Bierbrauer and Phillips (2008), and the bubble dynamics studies of Lind and Phillips (2012, 2013).

The whole domain \( \Omega \) is filled with initially equally spaced particles - a specified number per unit area. Every marker particle \( p \) is initially located at a unique position \((x_p, y_p)\) and is assigned a colour, or identity, \( C_p \) defined by

\[
C_p = \begin{cases} 
1 & \text{if particle } p \text{ is in fluid } m, \\
0 & \text{if particle } p \text{ is not in fluid } m.
\end{cases}
\]

Assuming no change in phase, particles initially of fluid \( m \) will remain so indefinitely and will be advected with fluid \( m \). Hence, the colour function for each particle satisfies the advection equation, namely

\[
\frac{DC_p}{Dt} = 0.
\]

Eq. (14) is ensured through the Lagrangian update of the marker particles. As the particles remain of fluid \( m \), they can be assigned the constant material properties associated with fluid \( m \), such as fluid viscosities \( \mu_m \).

#### 3.3.1. Grid to particle interpolation

The marker particles, and hence the position of the relative phases, are updated using the velocities calculated on the Eulerian spectral element grid. The velocities are interpolated to each marker particle, and the particles are advected with these velocities according to

\[
\mathbf{u} = \frac{D\mathbf{x}}{Dt}.
\]

The benefits of a spectral element formulation mean that intermodal velocities can be found with ease and high accuracy using the Lagrange interpolants (Eq. (12a)). Therefore, a particle at \((x_p, y_p)\) can be easily and accurately assigned a velocity \( \mathbf{u}(x_p, y_p) \) and hence updated in position accordingly.

#### 3.3.2. Particle to grid interpolation

The material properties of the fluids, carried with the marker particles, need to be projected onto the grid before solving the governing equations for the next time step. Following Lind and Phillips (2012), material properties are assigned to each GLL node using the following averaging process:

\[
\phi_{i,j} = \sum_{m=1}^{M} \phi_m^{C_{i,j}}.
\]

where \( \phi_m \) denotes a material constant within fluid \( m \) (for example, viscosity) and \( M \) the total number of separate phases/fluids. Note that, in this article, we have three phases; the bubble, the adjacent fluid layer/cell and the ambient fluid. The quantity \( C_{i,j}^{C} \) is known as the interpolated colour function at the point \((i, j)\) and is given by

\[
C_{i,j}^{C} = \frac{\sum_{p} N_p S(x_p - x_i, y_p - y_j) C_p}{\sum_{p} N_p S(x_p - x_i, y_p - y_j)},
\]

where \( N_p \) is the total number of particles and \( S \) is a bilinear weighting function given by

\[
S(x - x_i, y - y_j) = \begin{cases} 
(1 - |\frac{x-x_i}{\Delta x}|)(1 - |\frac{y-y_j}{\Delta y}|) & \text{if } 0 \leq |\frac{x-x_i}{\Delta x}|, |\frac{y-y_j}{\Delta y}| \leq 1, \\
0 & \text{otherwise}.
\end{cases}
\]

Also, note that, by definition

\[
\sum_{m=1}^{M} C_{i,j}^{C} = 1.
\]

Although \( C_{i,j}^{C} \) is found by summing over all particles in the domain (Eq. (16)), only those within a square of area \( 4\Delta x\Delta y \) contribute to determining the interpolated colour function at GLL node \((i, j)\). The interpolated colour function will be weighted towards the colour function (Eq. (13)) of the majority of particles that are in close proximity to point \((i, j)\). Consequently, by Eq. (15), the material constants will be weighted towards those of the dominant fluid about \((i, j)\). Of course, this is important only in regions near the interface where two distinct fluid types are present. Within the bulk of fluid \( m = 1 \), \( C_{i,j}^{C} = 1 \) whereas \( C_{i,j}^{C} = 0 \) for all particles \( p \) near \((i, j)\). So \( C_{i,j}^{C} = 1 \) and \( C_{i,j}^{C} = 0 \); hence \( \phi_{i,j} = \sum_{m=1}^{3} \phi^{C_{i,j}^{C}} = \phi^1 \).

We have some choice in specifying the size of the search square \( 4\Delta x\Delta y \). For regular finite difference meshes, \( \Delta x \) and \( \Delta y \) are taken to be the regular grid spacings. However, the GLL points are unequally spaced. Consequently, it seems prudent to leave the size of the search square as an independent parameter, which can be altered to suit the problem at hand, under the restriction that

\[
\min (\Delta x_i, \Delta y) \leq \Delta x, \Delta y \leq \max (\Delta x_i, \Delta y).
\]

where \( \Delta x_i = |x_{i+1} - x_i|, i = 0, \ldots, N - 1 \) is the spacing between consecutive GLL points. In most instances, setting the search lengths \( \Delta x, \Delta y \) to be an average of \( \Delta x_i, \Delta y \) gives very reasonable results.

Note that throughout this article, we define additional marker particles \( \mathbf{x}_{\text{bot}}, \mathbf{x}_{\text{top}}, \mathbf{x}_{\text{top}} \), which do not interact with the fluid in any way but are used solely to track the positions of the bottom and top of the bubble, as well as a point initially central on the interface between the ambient fluid and adjacent fluid layer.

#### 3.3.3. Particle boundary conditions

It may be the case that particles near the boundary in the current time step may step outside the boundary in the next. To remedy this, the particles are simply reflected back into the domain by the amount at which they exceed it. This exact approach is used by Bierbrauer and Zhu (2007) in their finite difference study and by Lind and Phillips (2012).

#### 3.3.4. A comment on surface tension

Note that throughout this article, surface tension is neglected. Physically, when using our non-dimensionalisation with surface tension values based on the Definity® (Bristol Myers Squibb Medical Imaging, N. Billerica, MA, USA) ultrasound contrast agent (UCA) microbubble (see e.g. Sarkar et al., 2009), the Weber number is calculated as 3.6 and Capillary number is calculated as 0.12. So while
surface tension does not dominate bubble dynamics, it is physically significant. Its omission in this work partly results from the fact that surface tension has not yet been formally analysed within the marker particle framework; it is an open question whether the best approach is a particle-pairwise interaction force (mimicking molecular generation of surface tension, see e.g. Tartakovsky and Meakin, 2005) or a Continuum Surface Force (using the continuous colour function as devised by Brackbill et al. (1992)). This is a non-trivial body of work that deserves thorough investigation and the authors are working on this directly. Nevertheless, the results herein still provide useful insights into bubble-cell dynamics, with the absence of surface tension allowing isolation and clear observation of effects due to other important physics, such as viscoelasticity (see Section 6.2).

4. Validation

As is always the case for new numerical code, validation is required to ensure that the method works as expected. The SEMP method has been validated using a time-reversed rotation and multiphase Poiseuille flow examples which are discussed in Appendix C.1 and Appendix C.2, respectively. Here, we validate the bubble dynamics by considering a three-phase approximation to a two-phase example: bubble collapse near a rigid wall. This is accomplished by setting the fluid layer to have a high viscosity so that it approximates the rigid wall. This setup should obtain results that are in close qualitative agreement with the two-phase examples published by Lind and Phillips (2012). Throughout this section, let $\Omega = [0, 10]^2$ contain an initially circular bubble, with radius $R = 1$ and centre $\mathbf{x} = (5.0, 2.2)$ and a fluid layer $\Omega_\ell = [0, 10] \times [0, 1]$. We use the same parameters as those chosen by Lind and Phillips (2012); the bubble has density $\rho_{b,0} = \ln \rho_{b,0} = 0$ and viscosity $\mu_b = 10^{-4}$, while the ambient fluid has density $\rho_{f,0} = \ln(4)$ and viscosity $\mu_f = 10^{-2}$. The fluid layer density is given by $\rho_{\ell,0} = q_{f,0}$ whilst the viscosity is $\mu_\ell = 10^2$. The simulations were run until $T = 10$ with a time step length $\Delta t = 5 \times 10^{-3}$. The mesh used in this section is the same as the one used by Lind and Phillips (2012) and is depicted in Fig. 2a, where $N = 8$, $a_{\text{max}} = \rho_{\text{max}} = 9$. The initial configuration of this test case is shown in Fig. 3a.

Fig. 3b illustrates the colour function at the end of the simulation $t = T = 10$. Clearly, a broad jet has formed which impinges on the fluid layer and pushes the bubble contents out towards the side walls. Even though the viscosity of the fluid layer is very high, the centre of the fluid layer interface does move slightly upwards as the simulation progresses. Nevertheless, the results are in good qualitative agreement with the two-phase results of Lind and Phillips (2012) depicted in Fig. 3c.

5. Numerical investigation

This section is dedicated to the numerical investigation of the collapse of a gas-filled bubble near a fluid-fluid interface with a rigid backing, where both the ambient fluid and the fluid layer are Newtonian. As mentioned in the introduction, the SEMP method was developed for flows with small to moderate Reynolds number, or equivalently, when the density difference across phases is small. To the authors’ knowledge, these are the only results (experimental or numerical) for low inertia bubble collapse near a fluid-fluid interface backed by a rigid wall. In the interests of clarifying the effect of key parameters on dynamics, this section focuses primarily on the effect of viscosity, and accordingly omits any effects due to applied ultrasound, buoyancy or surface tension. In the Appendix A, we demonstrate that the bubble dynamics do not change under a $p$-refinement over a reasonable physical time $O(1)$ time units). Here, we consider variations in both the ambient fluid viscosity and the fluid layer viscosity by separating the results into two parts: when the ambient fluid viscosity is less than the fluid layer viscosity, $\mu_f < \mu_\ell$ and vice-versa, $\mu_f > \mu_\ell$. Finally, we consider the influence the rigid backing has on the collapse.

Throughout this section, the domain $\Omega = [0, 10] \times [0, 10]$ contains a gas-filled bubble, $\Omega_b$, and a fluid layer, $\Omega_\ell$, so that the ambient fluid occupies the domain $\Omega_f = \Omega \setminus (\Omega_b \cup \Omega_\ell)$. With the exception of Section 5.3, the bubble centre is positioned at $\mathbf{x} = (5, 2.2)$ with an initial radius $R = 1$. The bubble’s contents are modelled as a compressible fluid with log-density $q_{b,0} = 0$ and a
constant viscosity $\mu_b = 1 \times 10^{-5}$. The fluid layer occupies the domain $\Omega_z = [0, 10] \times [0, h]$, where a height $h = 1$ is assumed in all subsections except Section 5.3, and has the same density as the ambient fluid, i.e. $q_{z,0} = \ln(4) = q_{f,0}$. The time step length is given by $\Delta t = 5 \times 10^{-3}$. Note that $c^2 = 1000$.

5.1. Ambient fluid viscosity less than fluid layer viscosity

In this section we consider the case where the ambient fluid viscosity is less than the viscosity of the fluid layer. In this section we restrict ourselves to the time period $t = 0, \ldots, 0.5$, because, as indicated in Appendix A, the most interesting dynamics seem to occur within this period.

Fig. 4a–k (left column) illustrate the colour function, and specific velocity streamlines, at times $t = 0.04, 0.08, 0.12, 0.16, 0.2$ and 0.5 for material parameters $\mu_f = 10^{-3}$ and $\mu_c = 10^{-1}$. All the streamlines depicted in this section, and later in the article, were chosen during post-processing using Tecplot. The initial configuration is the same as depicted in Fig. 3a. At $t = 0.04$, the velocity streamlines clearly illustrate that the bubble has collapsed spherically, drawing the fluid-fluid interface upwards to the bubble. It will be shown later, that this initial collapse phase is controlled primarily by the pressure difference between the bubble and ambient fluid, with very little dependence on viscosity. The bubble then goes through an expansion phase which can be seen at $t = 0.08$ where the velocity streamlines clearly illustrates a tapering motion. This expansion pushes the centre of the fluid-fluid interface downwards slightly before the bubble is elongated towards the fluid-fluid interface (as a result of the tapering motion), which can be seen at $t = 0.12$. This elongation is commonly seen in bubble cavitation problems and may be accompanied by jet formation. No jet is seen here, however, due to rapid equilibration of pressures inside and outside the bubble after the initial collapse. The elongation of the bubble occurs due to a Bjerkes-style migration of the bubble (towards the more rigid layer). This migration causes the layer to compress slightly and then rebound, flattening the underside of the bubble at $t = 0.16$ and 0.2. From then on, the bubble dynamics approach a steady state, with no significant temporal change in dynamics. Small perturbations can be seen in the bubble surface at $t = 0.5$ (and more clearly in Fig. 5a). As mentioned, these arise due to an absence of surface tension, but may evolve into un-physical flow features at later times as their small scale is under-resolved by the grid. For larger viscosity values, these perturbations are dampened entirely (see Fig. 5) with long-term stability evident, as demonstrated in Fig. A21a.

Fig. 4b–l (right column) illustrate contours of the streamline normal stress at times $t = 0.04, \ldots, 0.5$. This stress is defined as the component of the Cauchy stress parallel to instantaneous streamlines, and provides a geometrically invariant measure of the normal stress in the direction of the flow (Bollada and Phillips, 2008). It is clear that the majority of normal stress occurs in the fluid layer region. In this article, we do not include the action of external forces such as gravity and therefore, the evolution of normal stress is caused solely by the bubble dynamics. At $t = 0.04$, a localised peak normal stress can be seen in the central bump in the fluid-fluid interface, before spreading throughout the fluid layer. Although this stress seems to dissipate as the simulation progresses, the fact that the stress is largest and highly localised in the early stages of dynamics has potential implications in biomedicine: if the fluid layer represents a cell or tissue layer, depending on the mechanical properties and biological response, this could be indicative of regions of damage or even cell death. It
Fig. 4. Illustration of colour function with velocity streamlines (left column) and streamline normal stress (right column), for $\mu_f = 10^{-3}$, $\mu_c = 10^{-1}$ at times $t = 0.04, \ldots, 0.5$. 
Fig. 4. Continued
is also evident that, as the simulation progress, the largest magnitudes of stress are seen at the rigid wall. We investigate the influence of the rigid wall later in the article, but note this may have significant implications for bubble cleaning processes (if the fluid layer were to be a model of some unwanted material deposit or contaminant).

5.2. Ambient fluid viscosity greater than fluid layer viscosity

In this section, we assume that the viscosity of the ambient fluid is greater than the viscosity of the fluid layer. Fig. 6 illustrates the colour function, and specific velocity streamlines, at times \( t = 0.2, 0.5, 10.0 \) for material parameters \( \mu_f = 10^{-1} \) and \( \mu_c = 10^{-3} \) (which are the opposite of the previous section). Plots of the colour function at times \( t = 0.04, \ldots, 0.16 \) have not been included as the motion of the bubble is remarkably similar to the previous section and therefore, the discussion for these times will not be repeated here. In the previous section, a near-steady state was attained (at \( t \approx 0.2 \)) where only small oscillations and migrations of the bubble were seen, but surface perturbations were visible due to small viscosities. Here, however, the bubble shape remains smoother at \( t = 0.2 \) and \( t = 0.5 \) due to the larger ambient viscosity and consequently, as discussed in the Appendix A, the simulation is able to run for much longer times. Fig. 6c illustrates the colour function at the later time of \( t = 10 \). It is clear that the fluid-fluid interface is continuing to push upwards into the bubble after its rebound; after all it now has a lower viscosity and better retains its momentum, initially generated by the bubble collapse in the earlier stages. It is clear from the velocity streamlines, that small vortices are created inside the bubble and also inside the fluid layer. \( \text{Brujan et al. (2001)} \) demonstrated that when a laser-generated cavitation bubble collapses near an elastic material (inertia dominated collapse), an ejection of the elastic material into the ambient fluid can be seen. A similar phenomenon is seen here, however due to the lower amount of inertia in these examples, the jet-like growth of the fluid-fluid interface does not pierce the bubble.

Fig. 7a illustrates contours of the streamline normal stress at times \( t = 0.04, 0.08, 0.12, 10. \) At \( t = 0.04 \), a relatively large amount of normal stress appears radially around the bubble as it collapses. This normal stress clearly dissipates outwards at \( t = 0.08 \) during the bubble expansion phase. However, note that there is a build up of normal stress between the bubble and the layer which again may have implications for cavitation erosion. Also notice that, as the simulation progresses, the normal stresses then dissipate outwards and partly into the fluid layer while decreasing in magnitude. Fig. 7d illustrates the normal stresses that are found at time \( t = 10 \). There is evidence of stress build-up on either side of the crest at the fluid-fluid interface. These stresses accompany the fluid mechanical motion that drives the interface upward. They are indicative of the retarding effect of the ambient fluid on the upwards jet, and also limit any possible penetration of the nearby bubble.

It is expected that increasing the viscosity of the layer would decrease the height of the fluid-fluid interface at \( t = 10 \). Indeed, this is illustrated in Fig. 8. As the dynamics are dominated by the pressure difference between the bubble and ambient fluid, the ef-
5.3. Fluid layer height investigation

This section is concerned with a numerical study of the influence of the rigid wall which backs the fluid layer. Analogous to the previous section, the domain Ω = [0, 10] × [0, 10] contains a gas-filled bubble, Ωb, and a fluid layer, Ωc, so that the ambient fluid occupies the domain Ωf = Ω \ (Ωb ∪ Ωc). The bubble centre is positioned at \( \bar{x} \) (which varies depending on the layer height) with an initial radius \( R = 1 \). The bubbles contents are modelled as a compressible fluid with log-density \( q_{b,0} = 0 \) and a constant viscosity \( \mu_b = 1 \times 10^{-5} \). The fluid layer occupies the domain \( \Omega_c = [0, 10] \times [0, h] \) (where the height is given by \( h = 0.3, 5.0 \)) and has the same density as the ambient fluid, i.e. \( q_{c,0} = \ln(4) = q_{f,0} \). The time step length is given by \( \Delta t = 5 \times 10^{-3} \). We separate our results into two parts: when the ambient fluid viscosity is less than the layer viscosity and vice-versa.

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**Fig. 7.** Streamline normal stress for \( \mu_f = 10^{-1}, \mu_c = 10^{-3} \) for \( t = 0.04, 0.08, 0.12, 10.0 \).

**Fig. 8.** Colour function for \( \mu_c = 10^{-3}, 10^{-2}, 10^{-1} \) when \( t = 10.0 \).
5.3.1. Ambient fluid viscosity less than fluid layer viscosity

Throughout this subsection, we let $\mu_f = 10^{-3}$ and $\mu_c = 10^{-1}$. A comparison of the colour function, density and streamline normal stress for the two cell heights quoted above, is considered. The density is plotted in place of the fluid pressure, on the understanding that the two are equivalent to within a multiplicative constant through the linear equation of state (2). By choosing a small and a large fluid layer height, $h$, we can easily assess the influence of the rigid wall backing the layer.

Fig. 9a and b illustrate a comparison of the colour function (and specific velocity streamlines) at interface heights $h = 0.3$ and 5.0. The plots are taken at time $t = 0.08$ as the majority of the dynamics occur early on the simulation. The difference in the bubble shape at the different heights is immediately obvious. At the smaller height, Fig. 9a, the bubble elongates towards the rigid wall where the velocity streamlines clearly illustrates a tapering motion (this behaviour was seen in the previous sections; see for example, Fig. 4c). Whilst at the larger height, Fig. 9b, the bubble collapses spherically as can be seen from the velocity streamlines. The reason for the substantial difference in bubble shapes can be immediately seen in the corresponding density contours illustrated in Fig. 9c and d. Fig. 9c shows that there is a region of lower pressure on the rigid wall in the region directly beneath the bubble. Due to the absence of buoyancy and surface tension, the pressure gradient is the driving force for the bubble elongation and migration towards the wall. On the other hand, at a greater height, Fig. 9d shows that the region of low pressure is contained in an annulus around the bubble, which dissipates outwards as the simulation progresses; meanwhile the bubble continues near-spherical oscillations of decreasing amplitude. Clearly, the fluid layer thickness is sufficiently large so as to minimise any effect of the wall on the bubble.

Fig. 9e and f illustrate the streamline normal stress at time $t = 0.08$ for heights $h = 0.3$ and 5.0, respectively. It is evident from Fig. 9e, that the normal stress is highest on the rigid wall, generated by the no-slip condition. This stress dissipates outwards along the rigid wall as the simulation progresses. For $h = 5.0$, Fig. 9f illustrates that the stress dissipates outwards in concentric circles in
a manner similar to the density/pressure, but with notably larger magnitudes found within the fluid layer. This is expected as the fluid layer is of a larger viscosity (by some two orders of magnitude).

5.3.2. Ambient fluid viscosity greater than fluid layer viscosity

Following on from the previous subsection, we swap viscosities and let \( \mu_f = 10^{-1} \) and \( \mu_c = 10^{-3} \). It was illustrated in an earlier section, that the increased ambient fluid viscosity increases the lifetime of the bubble. Therefore, Fig. 10a and b illustrate the colour function at time \( t = 7.0 \) at interface heights 0.3 and 5.0, respectively. Immediately, one sees the effect the rigid wall has on the fluid-fluid interface and bubble shape. At a height of \( h = 0.3 \), a jet forms in the fluid-fluid interface which is more rounded and elongated than at a height of \( h = 5.0 \). The fluid-fluid interface, at \( h = 0.3 \), penetrates a little further into the bubble when compared to the \( h = 5.0 \) case, most likely due to the increased pressure build up (and subsequent rebound driving force) in the smaller layer of fluid. Consequently, at the smaller height, the bubble can be seen to bend around the fluid-fluid interface much more significantly when compared to the larger height. It is known that when a bubble oscillates near a neighbouring cell, microstreaming is produced in the surrounding fluid (Wu, 2002). This microstreaming can be clearly seen in Fig. 10a and b. However, we note that there is very little production of shear stress associated with these microstreams due to their relative magnitude being small \( \approx O(10^{-2}) \).

In order to draw comparisons with the previous section, the streamline normal stress at time \( t = 0.08 \) is now considered. We do not consider comparisons for the colour function or density as results are found to be near-identical to the previous section for \( t \leq 0.08 \). Fig. 11a and b illustrate the streamline normal stress at interface heights 0.3 and 5.0, respectively, for time \( t = 0.08 \). Compared to the previous section, the largest build up stress is now seen in the ambient fluid. It is clear from Fig. 11a that there is a small build up of normal stress on the fluid-fluid interface which has possible implications for cell functionality, if the thin layer is representative of a thin cell layer. However, the same localised build-up is not clearly seen in Fig. 11b where the stress once again dissipates in concentric circles, but with magnitudes larger in the ambient fluid than the adjacent fluid layer. Note that we have not included plots of the normal stress contours at \( t = 7 \) because the stress is of negligible magnitude at this time for both heights.

6. Towards single cell-bubble interaction for sonoporation

One of the many applications of bubble dynamics is non-invasive and targeted drug delivery via sonoporation (Hernot and Klibanov, 2008; Lentacker et al., 2014; Wu and Nyborg, 2008). Drug-laden encapsulated microbubbles may be injected as a bubbly solution into the body, with ultrasound (applied at a desired location) acting to burst the bubbles and deliver the drug to the target site. Under the action of ultrasound, the bubble can collapse in two ways: so-called inertial (unstable) and non-inertial (stable) cavitation. The high speed liquid jet that tends to form in inertial cavitation may perforate the nearby cell (producing a pore in the cell membrane) and transport the drug into the cell through the perforation. It is not clear under what circumstances that the damage to the cell by the high speed liquid jet is usually repairable. Experiments by Hu et al. (2013), show that if the jet produces a high amount of cell perforation with a large pore size, then the cell will not repair itself. In contrast, non-inertial cavitation can be sustained at lower ultrasound intensities, causing the bubble...
to oscillate but not burst or produce a high speed jet. At these lower intensities, several mechanisms have been proposed which may enable drug uptake into the cell (Lentacker et al., 2014). It is possible that the oscillations of the bubble produce a pore in the cell membrane through the exertion of fluid mechanical stresses on the cell interface formed by the associated microstreaming flow (Wu, 2002). It is also possible that the bubble would migrate into, or directly push upon, the nearby cell due to the acoustic forcing (Lentacker et al., 2014). The above mechanical actions are in addition to biological processes where drug uptake may be achieved through endocytosis (the process by which cells absorb external molecules by engulfing them in their cell membrane). It is unknown which method produces the greater volume of drug delivery into the cell, but numerical simulations, such as those presented here, may offer important physical insights.

The results presented previously in this article, assume that the bubble is small in diameter in comparison to an adjacent fluid layer, which may model a large (locally flat) cell or a contaminant layer to be removed via microbubble cleaning. The diameter of cells in the human body can vary significantly, as can the diameter of microbubbles. For example, typically the diameter of an encapsulated microbubble used in conjunction with ultrasound, can vary between 1 – 10 μm (Cock et al., 2015). Therefore, this section presents the interaction between a bubble and a full suspended cell, where the two have similar spatial dimensions.

It was shown in the previous sections, that the interaction between the rigid wall and the bubble is dominant over the bubble-cell interaction. Therefore, our domain is chosen to be sufficiently large to negate any wall effects. Let \( \Omega = [0, 20] \times [0, 20] \) and assume that the bubble is situated directly on top of the cell where the centre point between the cell and the bubble is placed in the centre of the domain. The initial configuration is illustrated in Fig. 12b and the associated mesh is depicted in Fig. 12a below. The mesh parameters are: \( N = 10, \alpha_{\text{max}} = 12, \beta_{\text{max}} = 12 \). Initially, the adjacent cell will be modelled as a Newtonian viscous drop

(Section 6.1). However, in reality, cells will exhibit viscoelastic behaviour due to the various microstructures that are present in the cell’s interior. Therefore, we also consider a viscoelastic fluid approximation of the adjacent cell in Section 6.2.

6.1. Newtonian fluid

The dimensional and non-dimensional parameters used in this section are given in Table 1. To calculate the non-dimensional parameters, we employ the same scaling as given earlier in Section 2.1 where the initial bubble radius \( R = 1 \) μm, initial bubble density \( \rho_{b,0} = 1 \) kg · m\(^{-3} \) (⇒ \( q_{b,0} = 0 \)) and the reference speed of sound \( V = 3 \times 10^2 \) m · s\(^{-1} \) (the speed of sound through the air phase). The bubble, fluid and cell viscosities are of the (approximate) orders typically found for air, blood plasma and a red blood cell’s haemoglobin solution (see e.g. McClain et al., 2004), respectively. Note that the speed of sound parameter is taken to be \( c_0 = 1500 \) m · s\(^{-1} \).

Figs. 13–16 illustrate the colour function (with velocity streamlines), density contour, streamline normal and shear stresses at
In contrast to the previous sections, we wish to simulate an initial expansion phase (the likes of which would be seen when a bubble responds to a ultrasound wave trough). Thus, the initial density (and therefore, initial pressure) inside the bubble is taken to be larger than the density in the ambient fluid so that the bubble expands initially (Fig. 13a). The initial expansion, releases an approximately spherical pressure wave (Fig. 13b), into the surrounding fluid which dissipates fairly rapidly. This pressure wave induces a high in magnitude streamline normal stress at the top of the cell (Fig. 13c). As the bubble expands, it pushes into the nearby cell which causes a flattening of both the cell and the bubble, which can clearly be seen in Figs. 14a, 15a and 16a. At later times, the gap between the bubble and cell increases slightly due to the continuing expansion of the bubble pushing the cell downwards. As a result of the bubble expansion into the nearby cell, a region of high pressure develops, and persists, at the bottom of the bubble and top of cell surface (Figs. 14b, 15b and 16b). This persistent high pressure is reflected in the high normal stress region at the cell interface (Figs. 14c, 15c and 16c) which is sustained for the whole simulation, even as the normal stress elsewhere begins to spread and dissipate around the cell surface. Due to the normal stress being concentrated at a specific location in the cell, it could have potentially negative implications for cell functionality.

It is well known that during stable cavitation the oscillations of the bubble induce so-called microstreaming local to the bubble (see e.g. Lentacker et al., 2014; Wu, 2002). This microstreaming produces a shear stress (as well as a normal stress) on the
Fig. 14. Illustration of the colour function with velocity streamlines, density contour, streamline normal and shear stresses at time $t = 0.2$.

Membrane of the cell. Fig. 13d illustrates the build up of streamline shear stress on the fluid-cell interface. This shear stress is produced by the velocity field bending around the fluid-cell interface as can be seen in Figs. 15a and 16a. Figs. 15d and 16d illustrate that the shear stress spreads around the fluid-cell interface from towards the top of the cell to the middle, implying that a cavitation bubble can have a global effect on the cell. Leow et al. (2015), showed that so-called blebbing (a term used to describe a local distortion in the membrane of a cell) occurred, not only at the sonoporation site (e.g. the site of jet impact - inertial cavitation) but also along the membrane periphery. It was concluded that blebbing at the impact site may be involved in the cell’s repair process but no reasons are offered for the additional blebbing found along the membranes periphery. Leow et al. (2015) do indicate that non-local blebbing is quite likely, given that the actin cytoskeleton (a fibrous network in the interior of a cell which is connected to the cell membrane) is disrupted (see e.g. Chen et al., 2014). The results presented here illustrate spreading of both the normal and shear stresses along the cell membrane: a phenomenon purely hydrodynamical in nature. This raises the possibility that the hydrodynamical spreading of normal and shear stresses is the key mechanism in creating non-localised blebbing (and also non-local disruption of the actin cytoskeleton close to the cell membrane), rather than any biochemical cell response.

6.2. Viscoelastic fluid

In this section, we approximate the cell as a viscoelastic fluid; specifically an Oldroyd B fluid so that the extra-stress tensor
(Eq. (3)) can be supplemented by an additional term describing the polymeric stress contribution $\tau$, where the polymeric stress satisfies an additional constitutive law. The Oldroyd-B viscoelastic model is a natural choice due to its simplicity and previous usage within the compressible SEMF framework (Lind and Phillips, 2013). Thus, Eq. (3) becomes:

$$S = \eta_1^s \left( \nabla \mathbf{u} + \nabla \mathbf{u}^T \right) + \eta_2^s \left( \nabla \cdot \mathbf{u} \right) I + \tau,$$

where the polymeric stress $\tau$ satisfies a constitutive equation of (compressible) upper-convected Maxwell (UCM) type:

$$\tau + \lambda_1 \left( \ddot{\tau} + \left( \nabla \cdot \mathbf{u} \right) \tau \right) = \eta_1^p \left( \nabla \mathbf{u} + \nabla \mathbf{u}^T \right),$$

where the superscripts $s$ and $p$ denote the solvent and polymeric viscosities, respectively, and $\lambda_1$ denotes the characteristic relaxation time. The symbol $\ddot{\tau}$ denotes the upper-convected derivative and is defined by

$$\ddot{\tau} = \frac{D \tau}{D t} - (\nabla \mathbf{u}) \tau - \tau (\nabla \mathbf{u}^T).$$

Note that when $\eta_1^s = \eta_1^p = 0$, the Oldroyd-B model reduces to an upper-convected Maxwell (UCM) model. Employing the same non-dimensionalisation as that used in Section 2.1, introduces the Weissenberg number,

$$Wi := \frac{\lambda_1 V}{R},$$

as a non-dimensional measure of the fluid elasticity, for a given relaxation time. The numerical computation of viscoelastic fluids exhibits instabilities at high Weissenberg number (known as the high
Weissenberg number problem). However, no stabilization techniques are employed in this article. The non-dimensional constitutive equation for the polymeric stress is then given by

$$\tau + Wi\left(\nabla \cdot u + \nabla u^T\right) = \eta_p^\ast (\nabla u + \nabla u^T)$$

(23)

For further information regarding the viscoelastic constitutive equation given in Eq. (20), and its equivalent log-density formulation, the reader is referred to Lind and Phillips (2013).

In this section, the non-dimensional parameters for the bubble, ambient (Newtonian) fluid and solvent (Newtonian) contribution to the viscoelastic cell, are the same as those given in Table 1. The non-dimensional parameters for the polymeric contribution to the viscoelastic cell are given by: $\mu_p^{\ast} = 1$ (kinematic polymeric viscosity) and $Wi_c,0 = 10$ (Weissenberg number). Given values for cell elasticity quoted in the numerical study of Khismatullin and Truskey (2004) (where the values were taken from experiments), we choose a Weissenberg number close to the largest allowed by the method before the high Weissenberg numerical instability destroys the solution.

Figs. 17–20 illustrate the streamline polymeric normal stress and streamline polymeric shear stress at times $t = 0.1, \ldots, 0.5$. Note that the colour function, density contours, streamline solvent normal and shear stresses are omitted here as they are near-identical to the Newtonian case depicted in Section 6.1. Analogous to the previous section (see e.g. Fig. 13b), the initial expansion releases an approximately spherical pressure wave, into the surrounding fluid which dissipates fairly rapidly. Fig. 17a and b illustrate the streamline polymeric normal and shear stresses, respectively, at $t = 0.1$.
For the choice of polymeric viscosity and Weissenberg number studied here, the magnitude of the normal and shear stresses are much smaller in Fig. 17a and b when compared to their Newtonian equivalents (Fig. 13c and d).

Once again, similar to the Newtonian case, as the bubble expands, it pushes into the nearby cell which causes a flattening of both the cell and the bubble (see e.g. Figs. 14a, 15a and 16a). Similar to Section 6.1, at later times the gap between the bubble and cell increases slightly due to the continuing expansion of the bubble pushing the cell downwards. As a result of the bubble expansion into the nearby cell, a region of high pressure develops, and persists, at the bottom of the bubble and top of cell surface (Figs. 14b and 15b). It can be seen from Figs. 18a, 19a and 20a that the highest magnitude of streamline normal stress occurs in a thin layer just inside the fluid-cell interface. Additionally, it can be seen that the normal stress spreads more evenly throughout the whole cell as the simulation progresses. Indeed, the presence of elasticity results in a more evenly distributed stress being sustained in the cell, resembling behaviour that might be expected from a connected internal micro-structure.

It was shown in the Newtonian case previously, that a streamline solvent shear stress develops close to the fluid-cell interface as a result of bending velocity streamlines (see e.g. Fig. 13d). A similar effect is demonstrated in the streamline polymeric shear stress as
7. Conclusions and future work

In this article, we have extended the spectral element marker particle (SEMP) method to incorporate a third-phase. The full compressible, two-dimensional governing equations are solved using the spectral element method, whilst the three fluid phases are tracked using the marker particle method - a scheme that bears a strong resemblance to VOF methods. The marker particle method was validated using a time-reversed rotation (see Appendix C.1), where it was evident that the method exhibited approximately linear convergence with respect to increasing marker particle density. A satisfactory result given the highly complex three-phase distor-
tion observed. The SEMP method was then validated on two examples: a three-phase steady-state Poiseuille flow example (see the Appendix C.2) and bubble collapse near a highly viscous fluid-layer (which approximates a rigid wall). For the Poiseuille flow example, good qualitative agreement could be seen between the analytical and computed velocity solutions. However, the \( \nu \) component of the velocity field contained non-zero components which were attributed to an unavoidable smoothing error, present due to the continuous (smoothed) material parameters across the fluid-fluid interfaces. Nevertheless, a reasonable value of the maximum norm error between the analytical and computed velocity was given after long simulation times. The three-phase bubble collapse near a highly viscous fluid-layer gave good qualitative agreement with the two-phase bubble collapse near a rigid wall case presented by Lind and Phillips (2012).

A numerical investigation of low-inertia bubble collapse backed by a rigid wall was then presented. In the Appendix A, it was illustrated that SEMP exhibited mesh independence (under \( p \)-refinement for reasonable time-scales (O(1) time units)). A numerical study of the influence of viscosity was then undertaken, with various values and combinations considered, including cases when the ambient fluid viscosity is greater than the fluid layer, and vice versa. When the ambient fluid viscosity is less than the fluid layer viscosity, a localised peak normal stress was seen in the central bump of the fluid-fluid interface. The fact that the normal stress is localised has potential implications for cell functionality. When the ambient fluid viscosity is greater than the fluid layer viscosity, the simulation remained stable for larger computational times. At larger times, the fluid layer continued pushing upwards into the bubble as a result of better momentum retention in the layer. At these later times, there was evidence of stress build up on either side of the crest of the fluid-fluid interface. These stresses are indicative of a retarding effect of the ambient fluid on the upwards motion of the fluid-fluid interface. Vortices were shown to be present in the fluid layer at these later times. An investigation of the height between the fluid-fluid interface and the rigid wall which backs the fluid-cell was then presented. It was shown that the bubble collapsed spherically at larger interface heights from the rigid wall as result of the reduced interaction between the bubble and the rigid wall.

A (simplified) bioengineering example was considered, where a bubble was placed near a cell. The cell was approximated first as a Newtonian viscous drop and then as an Oldroyd B viscoelastic fluid. The viscous drop was assumed to have material parameters typical of air, blood plasma and a red blood cell haemoglobin solution. A region of high pressure developed at the cell surface as a result of the interaction between the cell and bubble, and this persisted for the duration of the simulation. Initially, a high amount of normal stress was seen to build up at the top of the cell and this then spread out along the cell interface. Similar behaviour was also seen for the shear stress where the shear stress is caused by the bending of velocity streamlines around the cell. The polymeric normal stress, although lower in magnitude than the solvent counterpart, spreads more evenly throughout the interior of the cell illustrating behaviour expected of the internal cell microstructure. The polymeric shear stress was seen to spread out along the cell interface in a much thinner layer than the solvent counterpart. The fact that the normal and shear stresses spread out along the cell interface is a potential reason for the non-localised blebbing phenomenon seen as a cell membrane recovers post bubble/ultrasound interaction (Leow et al., 2015).

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Appendix A. Mesh choice
A \( p \)-refinement study of Mesh 2 (depicted in Fig. 2b) is undertaken for a bubble placed near a fluid layer. Similarly to Section 4, the simulation is run until \( t = T = 10 \) with a time step length \( \Delta t = 5 \times 10^{-3} \).

For viscosities \( \mu_f = 10^{-1} \), \( \mu_c = 1.0 \), the mesh demonstrates near independence in the position markers with \( p \)-refinement for long physical times (see Fig. A21a). This helps to confirm that for parameter values of this order, long simulations may be run with some confidence in the accuracy of the results. For an ambient fluid viscosity some two orders of magnitude smaller \( \mu_f = 10^{-3} \), converged solutions are obtained over a shorter timescale, with near independence in \( p \)-refinement demonstrated up to \( t = 1 \) (see Fig. A21b). Beyond this, results lose grid independence, as small scale perturbations in the bubble surface, which are sensitive to grid resolution, grow undamped by any viscous or surface tension effects. Accordingly, the physical time of \( t = 1 \) will be deemed the approximate limit for reliable, grid independent solutions when \( \mu_f = 10^{-3} \). This restriction at lower viscosity has little impact on the applicability of the method as it is often the case (at lower viscosities) that the most interesting and important bubble dynamics are at the start of the growth/collapse process, before any potential steady states are reached.

Note that over the time scales considered in subsequent sections of this article, the solutions also displayed mesh independence between Mesh 1 and Mesh 2 (depicted in Fig. 2). However, the comparison is not included here in the interests of brevity.

Appendix B. Analytical solution for three-phase steady-state Poiseuille flow
We derive the analytical solution for steady-state Poiseuille flow of three adjacent immiscible fluids. This derivation follows the solution of Bird et al. (2007) for two-phase Poiseuille flow. Consider three immiscible, incompressible fluids flowing in the \( x \) direction in a horizontal thin slit of length \( L \) and height \( H \) under the influence of a horizontal pressure gradient \( \partial p/\partial x = P \). Thus, we define our domain \( \Omega = [0, L] \times [0, H] \), which contains three distinct phases: \( \Omega_1 = [0, L] \times [0, a] \), \( \Omega_2 = [0, L] \times [a, b] \) and \( \Omega_3 = [0, L] \times [b, H] \). The liquid phases are flowing sufficiently slowly so that the fluid-fluid interfaces remain planar. Note that the fluids in each phase have distinct viscosities, \( \eta_1, \eta_2 \) and \( \eta_3 \).

The equations governing incompressible fluid motion are given by

\[
\rho \frac{Du}{Dt} = -\nabla p + \nabla \cdot \mathbf{S},
\]  
\[\nabla \cdot \mathbf{u} = 0,\]  
\[\mathbf{S} = \eta (\nabla \mathbf{u} + \nabla \mathbf{u}^T),\]  

where \( \rho \) is the density, \( \mathbf{u} \) is the velocity, \( \eta \) is the viscosity, \( p \) is the pressure, and \( \mathbf{S} \) is the deviatoric stress tensor.
where $\rho$ is the constant density, $\eta$ is the constant viscosity, $\mathbf{u}$ is the velocity, $p$ is the pressure and $\mathbf{S}$ is the extra-stress tensor. In addition to the constant pressure gradient in the $x$ direction, steady-state Poiseuille flow assumes that the pressure is a function of $x$ alone, $p = p(x)$, that the velocity field has the form $\mathbf{u} = (u, y) = (u(y), 0)$ and that there is no time-dependence $\partial / \partial t = 0$. Thus, in component form, Eq. (B.1a) reduces to

$$0 = -p + \frac{\partial S_{xx}}{\partial x} + \frac{\partial S_{xy}}{\partial y} \quad (B.2a)$$

$$0 = \frac{\partial S_{xy}}{\partial x} + \frac{\partial S_{yy}}{\partial y} \quad (B.2b)$$

Note that the incompressible constraint (B.1b) is automatically satisfied by the assumption on the velocity field. The components of the extra-stress tensor (Eq. (B.1c)) are given by

$$S_{xx} = 0, \quad S_{xy} = \eta \frac{\partial u}{\partial y} = S_{yx}, \quad S_{yy} = 0 \quad (B.3)$$

Substituting the extra-stress components (Eq. (B.3)) into Eqn. (B.2a) causes the $y$ component of the momentum equation (Eq. (B.2b)) to vanish and the $x$ component (Eq. (B.2a)) reduces to

$$\frac{\partial S_{xy}}{\partial y} = p \quad (B.4)$$

Eq. (B.4) holds for each phase $i = 1, 2, 3$. Thus, integrating Eq. (B.4) with respect to $y$ yields

$$S_{xy}^i = Py + C_i^1, \quad (B.5)$$

where $i = 1, 2, 3$ denotes each fluid phase and the arbitrary coefficients of integration $C_i^1$ are constant because $S_{xy}$ has no dependence on $x$. According to Bird et al. (2007), the shear stress must be continuous across each fluid-fluid interface. Thus, we have two boundary conditions on the shear stress

$$S_{xy}^1 = S_{xy}^2 \quad \text{when} \quad y = a, \quad (B.6a)$$

$$S_{xy}^2 = S_{xy}^3 \quad \text{when} \quad y = b. \quad (B.6b)$$

where $y = a$ and $y = b$ denote the interfaces between the fluid phases. Applying the boundary conditions (B.6) to the shear stress (Eq. (B.5)) for each phase tells us that $C_1^1 = C_2^1 = C_1^2 = C_3^3$. Using the definition of the shear stress, Eq. (B.5) becomes

$$\frac{\partial u_i}{\partial y} = \frac{p}{\eta_i} y + C_i^1, \quad (B.7)$$

where $u_i$ denotes the $x$ component of the velocity field for fluid $i$ and $\eta_i$ is the viscosity of fluid $i$, $i = 1, 2, 3$. Integrating Eq. (B.7) throughout with respect to $y$ yields

$$u_i = \frac{1}{2\eta_i} y^2 + \frac{C_i^1}{\eta_i} y + C_i^2, \quad (B.8)$$

for each fluid phase $i$. We have four coefficients which need to be determined; fortunately, we have four boundary conditions on the velocity:

$$u_1 = 0 \quad \text{when} \quad y = 0, \quad (B.9a)$$

$$u_1 = u_2 \quad \text{when} \quad y = a, \quad (B.9b)$$

$$u_2 = u_3 \quad \text{when} \quad y = b, \quad (B.9c)$$

$$u_3 = 0 \quad \text{when} \quad y = H \quad (B.9d)$$

Applying Eq. (B.9a) to Eq. (B.8) with $i = 1$ tells us that $C_1^1 = 0$. Similarly, applying the other boundary conditions on the velocity to Eq. (B.8) for each phase $i$ yields

$$\frac{p a^2}{2\eta_1} + \frac{C_1^1 a}{\eta_1} = \frac{p a^2}{2\eta_2} + \frac{C_2^1 a}{\eta_2} + C_2^2, \quad (B.10a)$$

$$\frac{p b^2}{2\eta_2} + \frac{C_2^1 b}{\eta_2} + C_3^2 = \frac{p b^2}{2\eta_3} + \frac{C_3^1 b}{\eta_3} + C_3^3, \quad (B.10b)$$

$$\frac{p H^2}{2\eta_3} + \frac{C_3^1 H}{\eta_3} + C_3^2 = 0 \quad (B.10c)$$

Fig. A21. $y$ coordinate of the position of the markers particles $x_{i0x}$, $x_{i0y}$ and $x_{i0z}$ in time for $\mu_c = 1.0$ using (a) $\mu_f = 10^{-1}$ and (b) $\mu_f = 10^{-3}$ when $\alpha_{max} = \beta_{max} = 9$ and $N = 8, 10, 12$. 

(a) $\mu_f = 10^{-1}$

(b) $\mu_f = 10^{-3}$
Immediately, it can be seen that Eqs. (B.10a) and (B.10c) can be rearranged to write $C_2^3$ and $C_2^4$ in terms of $C^1$. Substituting these into Eq. (B.10b) yields an expression for $C_1$. Once $C_1$ is known, then $C_2^3$ and $C_2^4$ can be determined from Eqs. (B.10a) and (B.10c). Therefore, the three-phase steady-state Poiseuille flow solution is given by

$$C^1 = \left[ \frac{Pa}{2\eta_1} + \frac{Pa^2}{\eta_1} (b^2 - a^2) + \frac{P}{\eta_1} \left( H^2 - b^2 \right) \right] \left( \frac{1}{\eta_1} (a - b) + \frac{1}{\eta_1} (b - H) - \frac{a}{\eta_1} \right),$$  \hspace{1cm} (B.11a)

$$C_2^2 = \frac{Pa^2}{2\eta_1} + \frac{C_1^a}{\eta_1} - \frac{Pa^2}{2\eta_2} - \frac{C_1^a}{\eta_2},$$  \hspace{1cm} (B.11b)

$$C_2^2 = - \frac{PH^2}{2\eta_3} - \frac{C^1 H}{\eta_3},$$  \hspace{1cm} (B.11c)

$$u_1(y) = \frac{P}{2\eta_1} y^2 + \frac{C_1}{\eta_1} y + C_2^1,$$  \hspace{1cm} (B.11d)

$$u_2(y) = \frac{P}{2\eta_2} y^2 + \frac{C_1}{\eta_2} y + C_2^2,$$  \hspace{1cm} (B.11e)

$$u_3(y) = \frac{P}{2\eta_3} y^2 + \frac{C_1}{\eta_3} y + C_2^3.$$  \hspace{1cm} (B.11f)

It is straightforward to show that the analytical solution given in Eq. (B.11) remains valid for the log density formulation used in this article.

**Appendix C. Additional validation**

The numerical method is validated using the case of three-phase time-reversed rotation, in addition to a three-phase Poiseuille flow example. Throughout this section, the following error measure for the phase mass used is:

$$E_m^m = |M_m^m - M_m^m|.$$  \hspace{1cm} (C.1)

where $M_m^m$ and $M_m^{m_r}$ are given by

$$M_m^{m_r} = \int \Omega d\Omega, \quad M_m^m = \int \Omega d\Omega.$$  

Note that the fluid phases are identified by $m = 1, 2, 3$. Additionally, for the steady state three-phase Poiseuille flow example considered in Appendix C.2, the error of the velocity profile with respect to the $L^2$ and maximum norms is also used to validate the SEMP method:

$$\|u - u_N\|_2 = \left( \int \Omega |u - u_N|^2 d\Omega \right)^{1/2},$$  \hspace{1cm} (C.2a)

$$\|u - u_N\|_\infty = \max_{x \in \Omega} |u(x) - u_N(x)|.$$  \hspace{1cm} (C.2b)

where $u$ and $u_N$ are the analytical and computed velocity profiles, respectively.

**C1. Time reversed rotation**

Although the marker particle method has been validated for two-phase simulations (Lind and Phillips, 2012), the presence of an additional phase makes it necessary for re-validation. Let $\Omega = [0, 1]^2$ contain an initially circular bubble with radius $R = 0.15$ and centre $x = (0.5, 0.75)$, with an adjacent fluid layer $\Omega_c = [0, 1] \times [0, 0.1]$. The initial configuration is depicted in Fig. C.22a. The fluid is then advected according to a velocity field $u(x, t)$, whose time-dependent components are given by

$$u(x, y, t) = -\sin(2\pi y) \sin^2(\pi x) \cos \left( \frac{\pi t}{T} \right).$$  \hspace{1cm} (C.3a)

Table C2

<table>
<thead>
<tr>
<th>$N_p$</th>
<th>$E_m^m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m = 1$</td>
<td>$m = 2$</td>
</tr>
<tr>
<td>$301^2$</td>
<td>$1.17 \times 10^{-4}$</td>
</tr>
<tr>
<td>$401^2$</td>
<td>$1.76 \times 10^{-4}$</td>
</tr>
<tr>
<td>$501^2$</td>
<td>$9.94 \times 10^{-5}$</td>
</tr>
<tr>
<td>$601^2$</td>
<td>$4.56 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

where $t \in [0, T]$ and $T$ is the final time of the simulation. The velocity field (C.3) will reverse at time $t = T/2$ and return to its initial position at $t = T$. An illustration of the deformation undergone by both the bubble and the fluid layer, at $t = T/2$, is depicted in Fig. C.22b.

There are two ways to increase the marker particle density; increasing the number of particle cells in each direction ($N_x$, $N_y$) (akin to $h$-refinement), or increasing the number of particles per-cell $N_p$ (akin to $p$-refinement). The minimum distance between Gauss-Lobatto Legendre points scales with $O(1/N^2)$, approximately. Therefore, when $N = 10$, we require $N_x$, $N_y \leq 100$ so that Eq. (18) is satisfied. Thus, we set $N_x = N_y = 100$ and consider increasing the marker particle density by increasing $N_p$.

Table C2 shows the error in the mass at the end of the simulation, $t = T$, for a single mesh with increasing marker particle density, and for each phase $m = 1, 2, 3$. It is evident that increasing the marker particle density improves the mass error with approximate linear convergence seen in most cases. This is a satisfactory result, especially given the highly complex three phase distortion observed for this test case.

**C2. Multiphase Poiseuille flow**

The three-phase spectral element marker particle method (SEMP) is validated using a steady state Poiseuille flow example. Following Appendix B, consider three immiscible, incompressible fluids flowing in the $x$ direction in a horizontal thin slit of length $L$ and height $H$ under the influence of a horizontal pressure gradient $\partial P/\partial x = P$. Thus, we define our domain $\Omega = [0, L] \times [0, H]$, which contains three distinct phases:

$$\Omega_1 = [0, L] \times [0, a], \quad \Omega_2 = [0, L] \times [a, b] \quad \text{and} \quad \Omega_3 = [0, L] \times [b, H],$$

where $a = H/3$ and $b = 2H/3$. Note that throughout this subsection, $L = 10$ and $H = 5$. The liquid phases are flowing sufficiently slowly so that the fluid-fluid interfaces remain planar. Note that as the analytical solution assumes incompressibility, the speed of sound is increased to a very large value ($c^2 = 10^9$), and the dilatational viscosity given in (3) is set to zero. Each fluid phase is assumed to have distinct dynamic viscosities, defined as $\eta_1$, $\eta_2$, and $\eta_3$, where the subscripts are not to be confused with the subscripts in (3). The analytical solution for two-phase steady state Poiseuille flow is given by Bird et al. (2007). However, in the absence of a three-phase steady state Poiseuille flow solution, the authors have provided a derivation which is available in Appendix B.

In this section, we set $c^2 = 10^9$, $\mu_1 = 5$, $\mu_2 = 3$ and $\mu_3 = 8$ and run the simulation for 10,000 time steps with a time step length $\Delta t = 10^{-4}$, so that $T = 1$. A uniform, quadrilateral mesh is employed in this section with parameters $\alpha_{\text{max}} = 10$, $\beta_{\text{max}} = 10$ and $N = 8, 10$. The initial and boundary conditions for the velocity field are taken to be the analytical solution. For the viscosities considered in this section, Fig. C.23a and b illustrate the analytical and
computed $u$ components of the velocity field at the end of the simulation, respectively, when $N = 10$. Clearly good qualitative agreement is seen between the analytical and computed velocity solutions. The contour plots are the magnitudes of the $v$ component of the velocity field. The analytical $v$ component should be identically zero, as can be seen in Fig. C23a. However, it is clear from Fig. C23b, that the computed solution contains small non-zero contributions to the $v$ component around the interface between the phases. The non-zero $v$ component in the computed solution is an error introduced by the smoothing of the material parameters across the interface between phases which, theoretically, contains a weak discontinuity (due to different viscosities). This error is an unavoidable consequence of adopting a “one field” model, but is clearly small in magnitude ($\approx 2 \times 10^{-2}$) and little cause for concern.

To confirm that the method is indeed converging to the analytical solution, we carry out a $p$-type convergence study. Every time the polynomial degree is increased, or the mesh width decreased, the number of marker particle cells $N_x$ and $N_y$ must also be increased to ensure a decreasing width of the interface region with refinement. We define the marker particle mesh width $\Delta x = L/N_x$ and $\Delta y = H/N_y$. Therefore, given that the minimum distance between the GLL points scales as $O(1/N^2)$ and the maximum distance scales as $O(1/N)$, we define $N_x$ and $N_y$ as

$$N_x = \left\lfloor \frac{L(N + 1)}{2} \right\rfloor$$

$$N_y = \left\lfloor \frac{H(N + 1)}{2} \right\rfloor$$

which guarantees that (18) is satisfied. It can be seen from Fig. C24a and b that for $N = 8, 10$ and 12, the convergence is monotonic and of a high rate $\approx 3$. Note that the $x$ and $y$ components have been considered separately. This is excellent considering that this problem is a complex one: the analytical velocity field contains a weak discontinuity across the interface between each phase which is smoothed, using the interpolated colour function. This ob-
viously, introduces an unavoidable error into the method. Additionally, the interpolated colour function is calculated by interpolating a discrete (particle) colour function which is based on the position of the particles which are updated in time. This, therefore, introduces both interpolation and temporal error. The compounding of these errors, explains the relatively high error magnitudes observed at low resolutions.

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