

A BOUNDARY INTEGRAL FORMULATION FOR COMPRESSIBLE STOKES FLOW

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Abstract. *The interplay between viscous and surface tension and its influence on the evolving emulsion microstructure during its expansion is fundamental to the science and technology of emulsion processing. This article describes a general boundary integral formulation for compressible Stokes flows. The approach is then applied for 3D simulations of emulsion densification with periodic boundary conditions that involves an uniform expansion of a viscous fluid containing spherical drops on a body centered cubic lattice (BCC).*

Key- Words: *Boundary Integral, Compressible, Emulsion, Densification*

1. INTRODUCTION

The dynamics of interface deformation in low Reynolds number flow is of interest in a wide variety of fields including chemical and petroleum engineering, solid-earth geophysics, hydrology and biology. Typical applications span an immense range of length scales from microns to hundreds of kilometers: biological studies of cell deformation; chemical engineering studies of coalesce, flotation, coating flows and the dynamics of thin films. In the low Reynolds number limit the motion is governed by the Stokes and continuity equations. Although time-dependence does not appear explicitly in Stokes equations, it is consistent to study time-dependent interface deformation. This quasi-static assumption requires that the time scale for the diffusion of vorticity ℓ^2/ν , where ν is the kinematic viscosity and ℓ characteristic length of the flow, is much less than a typical time scale for a drop in an emulsion deform significantly, $\ell\mu/\Gamma$. Here Γ is surface tension.

The boundary integral method relates velocities at points within the fluid to the velocity and stress on the bounding surfaces. It is an ideal method for studying free-boundary problems (Pozrikidis 1992). Advantages of the technique include the reduction of the problem dimensionality, the direct calculation of the interfacial velocity, the ability to track large surface deformations, and the potential for easily incorporating interfacial tension. The integral equation method was first implemented numerically by Rallison & Acrivos (1978). In recent

years the number of applications including simulations of dilute and concentrated emulsion has increased enormously (Rallison 1984; Loewenberg & Hinch 1996; Cunha, Neimer, Blawdziewicz & Loewenberg 1999 and Cunha & Loewenberg 1999).

This work proceeds by considering the extension of the boundary integral formulation for compressible Stokes flows. We provide some of the details of the basic integral equations, along with the original modifications necessary for the study of dense emulsions. We use a mesh restructuring algorithm that is adaptive to the instantaneous surface configuration. For deformable drops, mesh restructuring is based on a curvature-rule, and is fully independent from the history of deformation (velocity calculations). A gap-rule is also implemented when near contact motion of interacting drops needs to be accurately resolved. In the last part of the article, we outline the numerical techniques typically applied in densification of emulsions .

2. BALANCE EQUATIONS AND BOUNDARY CONDITIONS

The theoretical formulation discussed here will be applied to investigate densification of emulsions formed by drops of viscosity $\lambda\mu$ and radius a (undeformed shape at $time = 0$) immersed in a second immiscible fluid of viscosity μ with an externally imposed velocity field \mathbf{u}^∞ . In the following analysis, we assume that the Reynolds numbers for the flows inside and outside the drop are both extremely small, $Re = \rho u^\infty a / \mu$, $Re = \rho u^\infty a / \lambda\mu \ll 1$. It will be helpful to keep in mind that λ denotes the viscosity ratio between the internal and the external flow, and when $\lambda = 0$ or ∞ the particle becomes a frictionless bubble or a rigid body, respectively.

2.1. Governing Equations

In the regime of low Reynolds number, compressible fluid motions are governed by the Stokes and continuity equations

$$-\nabla \left(p - \frac{1}{3}\mu\Delta \right) + \mu\nabla^2 \mathbf{u} + \rho \mathbf{b} = \mathbf{0} \quad \text{and} \quad \nabla \cdot \mathbf{u} = \Delta, \quad (1)$$

Here, \mathbf{u} is the Eulerian velocity field, p is the pressure, μ and ρ are the fluid viscosity and density, respectively, \mathbf{g} is the gravitational acceleration, and $\Delta = V^{-1}DV/Dt$ is the rate of expansion of the flow.

2.2. Boundary Conditions

The boundary conditions on a drop interface S with surface tension Γ require a continuous velocity across the interface and a balance between the net surface traction and surface tension forces (Pozrikidis 1992) that express the discontinuity in the interfacial surface forces. Mathematically, these conditions are expressed as

$$\mathbf{u} \rightarrow \mathbf{u}^\infty \quad |\mathbf{x}| \rightarrow \infty; \quad \mathbf{u}(\mathbf{x}) = \mathbf{u}'(\mathbf{x}), \quad \mathbf{x} = \mathbf{x}_i \in S \quad (2)$$

and the constitutive equation for an active interface free of surface viscosity, surface elasticity and surface module of bending and dilatation, the traction jump $[\mathbf{n} \cdot \boldsymbol{\sigma}]$ is given by Pozrikidis (1992)

$$\Delta \mathbf{t} = [\mathbf{n} \cdot \boldsymbol{\sigma}] = \kappa \Gamma \mathbf{n} - (\mathbf{I} - \mathbf{nn}) \cdot \nabla \Gamma. \quad (3)$$

It should be important to note that $(\mathbf{I} - \mathbf{nn}) \cdot \nabla$ denotes the gradient operator ∇^s tangent to the interface, \mathbf{I} is the identity tensor and \mathbf{n} is the unit normal vector to S . $\nabla^s \cdot \mathbf{n}$ defines the mean

curvature of the interface κ . In general, it can be expressed as the sum of the inverse principal radii of curvature $\kappa = R_1^{-1} + R_2^{-1}$. A kinematic constraint relates changes in the interface position to the local velocity. The interface evolution may be described with a Lagrangian representation $D\mathbf{x}_i/Dt = \mathbf{u}(\mathbf{x}_i)$.

3. INTEGRAL FORMULATION

The boundary-integral formulation developed here provides a powerful method for computing compressible Stokes flow by solving integral equations for functions that are defined over the boundaries. The important benefits of this extended approach is the ability to track deformation and swelling of drops in concentrated emulsions.

3.1. Reciprocal Theorem for a Newtonian Fluid

The reciprocal identity find extensive applications in the study of Stokes Flows. The major strength of the reciprocal identity is that it allows us to obtain information about a flow without having to solve the equations of the motion explicitly, but simply by using information about another flow (Happel & Brenner 1983). Consider a closed region of fluid V bounded by a surface S . Now consider two unrelated compressible flows of two different Newtonian fluids with densities ρ and ρ' and viscosities μ and μ' , and stress fields $\boldsymbol{\sigma}$ and $\boldsymbol{\sigma}'$, respectively:

Flow 1: $\mathbf{u}, \boldsymbol{\sigma}; (\rho, \mu)$. The equations for conservation of mass and momentum in terms of the material derivative, D/Dt , for the flow 1 are respectively:

$$\nabla \cdot \mathbf{u} = \frac{1}{V} \frac{DV}{Dt} \quad (\text{balance of mass}), \quad \rho \frac{D\mathbf{u}}{Dt} = \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{b} \quad (\text{balance of momentum}). \quad (4)$$

Here, locally, \mathbf{u} is the velocity, $\boldsymbol{\sigma}$ is the stress field and \mathbf{b} is the external body force per unit of mass. The Newtonian constitutive equation for a compressible flow is given by $\boldsymbol{\sigma} = -p\mathbf{I} + 2\mu\mathbf{E} - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}$ (constitutive equation), where \mathbf{I} is the identity, and $\mathbf{E} = \frac{1}{2}(\nabla\mathbf{u} + \nabla^t\mathbf{u})$, is the rate of strain tensor.

Flow 2: $\mathbf{u}', \boldsymbol{\sigma}'; (\rho', \mu')$. Similarly, the conservation and constitutive equations for the flow 2 are respectively

$$\nabla \cdot \mathbf{u}' = \frac{1}{V'} \frac{DV'}{Dt}, \quad \rho' \frac{D\mathbf{u}'}{Dt} = \nabla \cdot \boldsymbol{\sigma}' + \rho' \mathbf{b}', \quad \boldsymbol{\sigma}' = -p'\mathbf{I} + 2\mu'\mathbf{E}' - \frac{2}{3}\mu'(\nabla \cdot \mathbf{u}')\mathbf{I}, \quad (5)$$

where $\mathbf{E}' = \frac{1}{2}(\nabla\mathbf{u}' + \nabla^t\mathbf{u}')$ is the rate of deformation for the fluid 2. First consider the tensorial operation

$$\boldsymbol{\sigma} : \mathbf{E}' = -p\mathbf{I} : \mathbf{E}' + 2\mu\mathbf{E} : \mathbf{E}' - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} : \mathbf{E}', \quad (6)$$

but for a Newtonian compressible flow $\mathbf{I} : \mathbf{E}' = \frac{1}{2}\mathbf{I} : (\nabla\mathbf{u}' + \nabla^t\mathbf{u}') = \nabla \cdot \mathbf{u}' = \Delta'$. Δ denotes the rate of expansion of the flow. Thus (6) may be writren as

$$\boldsymbol{\sigma} : \mathbf{E}' = -\left(p + \frac{2}{3}\mu\Delta\right) \Delta' + 2\mu\mathbf{E} : \mathbf{E}' \quad (7)$$

If the same steps are applied to $\boldsymbol{\sigma}' : \mathbf{E}$; it must reduce in an analogous fashion to

$$\boldsymbol{\sigma}' : \mathbf{E} = - \left(p' + \frac{2}{3} \mu' \Delta' \right) \Delta + 2\mu' \mathbf{E}' : \mathbf{E} \quad (8)$$

We require $\mathbf{E} : \mathbf{E}' = \mathbf{E}' : \mathbf{E}$ so that

$$\mathbf{E}' : \mathbf{E} = \frac{1}{2\mu} \left[\boldsymbol{\sigma} : \mathbf{E}' + \left(p + \frac{2}{3} \mu \Delta \right) \Delta' \right] \quad (9)$$

Now, substituting (9) into (8), ones obtain

$$\boldsymbol{\sigma}' : \mathbf{E} = - \left(p' + \frac{2}{3} \mu' \Delta' \right) \Delta + \frac{\mu'}{\mu} \boldsymbol{\sigma} : \mathbf{E}' + \frac{\mu'}{\mu} \left(p + \frac{2}{3} \mu \Delta \right) \Delta'. \quad (10)$$

As a consequence of the symmetry of the stress tensor $\boldsymbol{\sigma} : \nabla \mathbf{u}' = \underline{\boldsymbol{\sigma}}^t : \nabla \mathbf{u}' = \boldsymbol{\sigma} : \nabla^t \mathbf{u}'$. Then, one may write that

$$\boldsymbol{\sigma} : \mathbf{E}' = \boldsymbol{\sigma} : \nabla \mathbf{u}' = \nabla \cdot (\mathbf{u}' \cdot \boldsymbol{\sigma}) - \mathbf{u}' \cdot \nabla \cdot \boldsymbol{\sigma}. \quad (11)$$

In this step we make the dot product of Cauchy's equation (4) by \mathbf{u}' in order to define the last term in the RHS of 11. Therefore after substituting back the result of this operation into (11), it gives

$$\boldsymbol{\sigma} : \mathbf{E}' = \nabla \cdot (\mathbf{u}' \cdot \boldsymbol{\sigma}) - \rho \mathbf{u}' \cdot \frac{D\mathbf{u}}{Dt} + \rho \mathbf{u} \cdot \mathbf{b} \quad (12)$$

Reversing the role of the primed and unprimed variables, we obtain also

$$\boldsymbol{\sigma}' : \mathbf{E} = \nabla \cdot (\mathbf{u} \cdot \boldsymbol{\sigma}') - \rho' \mathbf{u} \cdot \frac{D\mathbf{u}'}{Dt} + \rho' \mathbf{u} \cdot \mathbf{b}' \quad (13)$$

Now, substituting (12) and (13) into (10), multiplying the resultant equation by μ and make few manipulations, one obtain an expression for the generalized Lorentz reciprocal theorem for low Reynolds number flow

$$\begin{aligned} \nabla \cdot (\mu \mathbf{u} \cdot \boldsymbol{\sigma}') - \nabla \cdot (\mu' \mathbf{u}' \cdot \boldsymbol{\sigma}) &= \rho \mu' (\mathbf{u}' \cdot \mathbf{b}) - \rho' \mu (\mathbf{u} \cdot \mathbf{b}') + \\ &+ \mu' \left(p + \frac{2}{3} \mu \Delta \right) \Delta' - \mu \left(p' + \frac{2}{3} \mu' \Delta' \right) \Delta \end{aligned} \quad (14)$$

3.2. Integral Representation for a Compressible Stokes Flow

Consider the particular flow of interest with velocity \mathbf{u} and stress tensor $\boldsymbol{\sigma}$. The known flow is the one due to a point force with strength \mathbf{h} , and located at a point \mathbf{x}_ρ . Suppose that the inertia of both fluids has a negligible influence on the motion of the fluid elements, and by convenience takes $\mu = \mu'$ and $\rho = \rho'$. Flow 1 and flow 2 for this particular situation are described as following.

Flow 1: \mathbf{u} , $\boldsymbol{\sigma}$. The equations for conservation of mass and momentum in terms of the material derivative, D/Dt , for the flow 1 are respectively: $\nabla \cdot \mathbf{u} = \Delta$ and $\nabla \cdot \boldsymbol{\sigma} = -\mathbf{B}$, where $\rho \mathbf{b} = \mathbf{B}$ is the body force by unit of volume and $\Delta = \nabla \cdot \mathbf{u}$ is the flow rate of expansion. $\boldsymbol{\sigma} = -p\mathbf{I} + 2\mu\mathbf{E} - \frac{2}{3}\mu\Delta\mathbf{I}$.

Flow 2: Fundamental solution of the Stokes Flow; \mathbf{u}' , $\boldsymbol{\sigma}'$. The fundamental solution for Stokes equations correspond to the velocity and stress fields at a point \mathbf{x} produced by

a point force \mathbf{h} located at \mathbf{x}_o :

$$\nabla \cdot \boldsymbol{\sigma}' = -\mathbf{B}' = \mathbf{h}\delta(\mathbf{x} - \mathbf{x}_o), \quad \nabla \cdot \mathbf{u}' = 0, \quad (15)$$

with $|\mathbf{u}'| \rightarrow 0$ and $|\boldsymbol{\sigma}'| \rightarrow \infty$ as $|\mathbf{x}| \rightarrow \infty$. The solution of such equations may be derived, for example, using Fourier transforms (Ladyzhenskaya 1969):

$$p'(\mathbf{x}) = -\frac{\mathbf{h}}{4\pi} \cdot \nabla \left(\frac{1}{r} \right); \quad \mathbf{u}'(\mathbf{x}) = \frac{1}{8\pi\mu} \mathbf{h} \cdot \mathbf{G}(\hat{\mathbf{x}}); \quad \boldsymbol{\sigma}'(\mathbf{x}) = -\frac{3}{4\pi} \mathbf{h} \cdot \mathbf{T}(\hat{\mathbf{x}}) \quad (16)$$

where, the stokeslet, \mathbf{G} and the stresslet \mathbf{T} are defined by the following expressions:

$$\mathbf{G}(\hat{\mathbf{x}}) = \frac{\mathbf{I}}{r} + \frac{\hat{\mathbf{x}}\hat{\mathbf{x}}}{r^3}; \quad \mathbf{T}(\hat{\mathbf{x}}) = \frac{\hat{\mathbf{x}}\hat{\mathbf{x}}\hat{\mathbf{x}}}{r^5}. \quad (17)$$

The above functions are the kernels or the free-space Green's functions that maps the force \mathbf{h} at \mathbf{x}_o to the fields at \mathbf{x} in an unbounded three-dimensional domain. Here $\hat{\mathbf{x}} = \mathbf{x} - \mathbf{x}_o$, and $r = |\hat{\mathbf{x}}|$. Physically $\mathbf{u} = \mathbf{G}(\hat{\mathbf{x}}) \cdot \mathbf{h}$ expresses the velocity field due to a concentrated point force $\mathbf{h}\delta(\mathbf{x} - \mathbf{x}_o)$ placed at the point x_o , and may be seen as the flow produced by the slow settling motion of a small particle. T_{ijk} is the stress tensor associate with the Green's function G_{ij} and $\sigma_{ik}(\mathbf{x}) = T_{ijk}h_j$ is a fundamental solution of the Stokes produced by the hydrodynamic dipole $\mathbf{D} \cdot \nabla \delta(\mathbf{x} - \mathbf{x}_o)$. $T_{ijk} = T_{kji}$ as required by symmetry of the stress tensor $\boldsymbol{\sigma}$

It is straightforward to show that Reciprocal Theorem for the present case (14), takes the form

$$\nabla \cdot (\mathbf{u} \cdot \boldsymbol{\sigma}') - \nabla \cdot (\mathbf{u}' \cdot \boldsymbol{\sigma}) = \mathbf{u}' \cdot \mathbf{B} - \mathbf{u} \cdot \mathbf{B}' - p' \Delta \quad (18)$$

Now, considering the body force exerted on the flow $(\mathbf{u}, \boldsymbol{\sigma})$ the gravity force $\mathbf{B} = \nabla(\rho\mathbf{g} \cdot \mathbf{x})$, substituting the expressions of the point-force solution into (18) and discarding the arbitrary constant \mathbf{h} ones obtain

$$\begin{aligned} -\frac{3}{4\pi} \nabla \cdot [\mathbf{u}(\mathbf{x}) \cdot \mathbf{T}(\hat{\mathbf{x}})] - \frac{1}{8\pi\mu} \nabla \cdot [\mathbf{G}(\hat{\mathbf{x}}) \cdot \boldsymbol{\sigma}(\mathbf{x})] &= \frac{1}{8\pi\mu} [\mathbf{G}(\hat{\mathbf{x}})(\rho\mathbf{g} \cdot \mathbf{x})] \\ &+ \mathbf{u}(\mathbf{x})\delta(\hat{\mathbf{x}}) + \frac{1}{4\pi} \nabla \left(\frac{1}{r} \right) \Delta. \end{aligned} \quad (19)$$

Note that we have used for the first term on the RHS of (19), the incompressibility of the singular solution $\nabla \cdot \mathbf{G} = 0$, so that $\mathbf{G} \cdot \nabla(\rho\mathbf{g} \cdot \mathbf{x}) = \nabla \cdot [\mathbf{G}(\rho\mathbf{g} \cdot \mathbf{x})]$. The above equation is valid everywhere except at the singular point x_o . Consider a material volume of fluid V bounded by the singly or multiply connected surface to evaluate the integration of (19). There are two situations to be considered next.

Point force outside V . For this case $\delta(\mathbf{x} - \mathbf{x}_o) = 0$ inside V and thus after integrating (19) the integral representation of the Reciprocal Theorem takes the form

$$\begin{aligned} -\frac{3}{4\pi} \int_V \nabla \cdot [\mathbf{u}(\mathbf{x}) \cdot \mathbf{T}(\hat{\mathbf{x}})] dV - \frac{1}{8\pi\mu} \int_V \nabla \cdot [\mathbf{G}(\hat{\mathbf{x}}) \cdot \boldsymbol{\sigma}(\mathbf{x})] dV &= \\ = \frac{1}{8\pi\mu} \int_V \nabla \cdot [\mathbf{G}(\hat{\mathbf{x}})(\rho\mathbf{g} \cdot \mathbf{x})] dV + \frac{\Delta}{4\pi} \int_V \nabla(r^{-1}) dV \end{aligned} \quad (20)$$

The volume integrals over V in (20) can be converted to the surface integrals over S , by using the divergence theorem obtaining

$$\begin{aligned} & \frac{1}{8\pi\mu} \int_S \mathbf{G}(\hat{\mathbf{x}}) \cdot \boldsymbol{\sigma}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) dS_x + \frac{3}{4\pi} \int_S \mathbf{u}(\mathbf{x}) \cdot \mathbf{T}(\hat{\mathbf{x}}) \cdot \mathbf{n}(\mathbf{x}) dS_x \\ & + \frac{1}{8\pi\mu} \int_S \mathbf{G}(\hat{\mathbf{x}})(\rho\mathbf{g} \cdot \mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) dS_x + \frac{\Delta}{4\pi} \int_S r^{-1} \mathbf{n}(\mathbf{x}) dS_x = \mathbf{0}, \end{aligned} \quad (21)$$

where \mathbf{n} is the unit outward normal to the surface S . Equation (21) is the integral representation of the flow if the singularity is outside V . We will show that the integral equation (21) is a useful identity for developing new integral equations in terms of jumps condition on the interface.

Point force inside V . In order to formally determine the integral representation for the situation which $\delta(\mathbf{x} - \mathbf{x}_o) \neq 0$ inside V , we must integrate again the equation (19). Applying the divergence theorem and δ -distribution property, one obtains

$$\begin{aligned} \mathbf{u}(\mathbf{x}_o) &= -\frac{1}{8\pi\mu} \int_S \mathbf{G}(\hat{\mathbf{x}}) \cdot \boldsymbol{\sigma}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) dS_x - \frac{3}{4\pi} \int_S \mathbf{u}(\mathbf{x}) \cdot \mathbf{T}(\hat{\mathbf{x}}) \cdot \mathbf{n}(\mathbf{x}) dS_x \\ &- \frac{1}{8\pi\mu} \int_S \mathbf{G}(\hat{\mathbf{x}})(\rho\mathbf{g} \cdot \mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) dS_x - \frac{\Delta}{4\pi} \int_S r^{-1} \mathbf{n}(\mathbf{x}) dS_x, \end{aligned} \quad (22)$$

Equation (22) is the integral representation of compressible Stokes in terms of four boundary distributions involving the Greens's functions \mathbf{G} , the stresslet \mathbf{T} and the potential source $1/r$. The first distribution on the RHS of (22) is termed the single-layer potential, the second distribution is termed double layer potential, whereas the last new term is a potential source distribution due to the compressibility of the flow with a constant rate of expansion.

3.3. Integral Representation in Terms of the Traction Jump

External flow representation. Using the reciprocal identity (21) for the internal flow \mathbf{u}' (inside the particle) at a point \mathbf{x}_o that is located exterior to the particle, one obtains

$$\begin{aligned} & \frac{1}{8\pi\mu} \int_S \mathbf{G}(\hat{\mathbf{x}}) \cdot \boldsymbol{\sigma}'(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) dS_x + \frac{3\lambda}{4\pi} \int_S \mathbf{u}'(\mathbf{x}) \cdot \mathbf{T}(\hat{\mathbf{x}}) \cdot \mathbf{n}(\mathbf{x}) dS_x \\ & + \frac{1}{8\pi\mu} \int_S \mathbf{G}(\hat{\mathbf{x}})(\rho'\mathbf{g} \cdot \mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) dS_x + \frac{\lambda\Delta'}{4\pi} \int_S r^{-1} \mathbf{n}(\mathbf{x}) dS_x = \mathbf{0}, \end{aligned} \quad (23)$$

Now, applying (22) for the external flow subject to \mathbf{u}^∞ , and combining the result with equation (23), the integral representation is obtained as a function of the traction jump $\Delta\mathbf{t}$,

$$\begin{aligned} \mathbf{u}(\mathbf{x}_o) &= \mathbf{u}^\infty(\mathbf{x}_o) - \frac{1}{8\pi\mu} \int_S \mathbf{G}(\hat{\mathbf{x}}) \cdot \Delta\mathbf{t}(\mathbf{x}) dS_x - \frac{3}{4\pi} \int_S [\mathbf{u}(\mathbf{x}) - \lambda\mathbf{u}'(\mathbf{x})] \cdot \mathbf{T}(\hat{\mathbf{x}}) \cdot \mathbf{n}(\mathbf{x}) dS_x \\ &- \frac{1}{8\pi\mu} \int_S \mathbf{G}(\hat{\mathbf{x}})(\Delta\rho\mathbf{g} \cdot \mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) dS_x - \frac{\Delta - \lambda\Delta'}{4\pi} \int_S r^{-1} \mathbf{n}(\mathbf{x}) dS_x, \end{aligned} \quad (24)$$

Internal flow representation. We repeat the above procedure for the internal flow. Hence, the integral representation of the internal flow is obtained when (22) is applied,

$$\begin{aligned} \mathbf{u}'(\mathbf{x}_o) &= \frac{1}{8\pi\lambda\mu} \int_S \mathbf{G}(\hat{\mathbf{x}}) \cdot \boldsymbol{\sigma}'(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) dS_x + \frac{3\lambda}{4\pi} \int_S \mathbf{u}'(\mathbf{x}) \cdot \mathbf{T}(\hat{\mathbf{x}}) \cdot \mathbf{n}(\mathbf{x}) dS_x \\ &+ \frac{1}{8\pi\lambda\mu} \int_S \mathbf{G}(\hat{\mathbf{x}})(\rho'\mathbf{g} \cdot \mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) dS_x + \frac{\Delta'}{4\pi} \int_S r^{-1} \mathbf{n}(\mathbf{x}) dS_x, \end{aligned} \quad (25)$$

Using the reciprocal identity (21) for the external flow \mathbf{u}' (outside the particle) at a point \mathbf{x}_o that is located interior to the particle, one obtains after dividing the full equation by λ , that

$$\begin{aligned} \frac{\mathbf{u}^\infty(\mathbf{x}_o)}{\lambda} - \frac{1}{8\pi\lambda\mu} \int_S \mathbf{G}(\hat{\mathbf{x}}) \cdot \boldsymbol{\sigma}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) dS_x - \frac{3}{4\pi\lambda} \int_S \mathbf{u}(\mathbf{x}) \cdot \mathbf{T}(\hat{\mathbf{x}}) \cdot \mathbf{n}(\mathbf{x}) dS_x \\ - \frac{1}{8\pi\lambda\mu} \int_S \mathbf{G}(\hat{\mathbf{x}})(\rho\mathbf{g} \cdot \mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) dS_x - \frac{\Delta}{4\pi\lambda} \int_S r^{-1} \mathbf{n}(\mathbf{x}) dS_x = 0. \end{aligned} \quad (26)$$

The integral representation of the internal flow as a function of the jump condition is obtained by combining (25) and (26)

$$\begin{aligned} \lambda\mathbf{u}'(\mathbf{x}_o) = \mathbf{u}^\infty(\mathbf{x}_o) - \frac{1}{8\pi\mu} \int_S \mathbf{G}(\hat{\mathbf{x}}) \cdot \Delta\mathbf{t}(\mathbf{x}) dS_x - \frac{3}{4\pi} \int_S [\mathbf{u}(\mathbf{x}) - \lambda\mathbf{u}'(\mathbf{x})] \cdot \mathbf{T}(\hat{\mathbf{x}}) \cdot \mathbf{n}(\mathbf{x}) dS_x \\ - \frac{1}{8\pi\mu} \int_S \mathbf{G}(\hat{\mathbf{x}})(\rho'\mathbf{g} \cdot \mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) dS_x - \frac{\Delta - \lambda\Delta'}{4\pi} \int_S r^{-1} \mathbf{n}(\mathbf{x}) dS_x, \end{aligned} \quad (27)$$

Integral representation for the interface. The integral representation for the flow solution at the interface is found by applying the jump condition $(1/2)[\mathbf{u}(\mathbf{x}_o) + \lambda\mathbf{u}'(\mathbf{x}_o)]$ to the equations (24) and (27). For the limit of \mathbf{x}_o going to the interface, $\mathbf{u}(\mathbf{x}_o) = \mathbf{u}'(\mathbf{x}_o)$ (continuity of velocity) and the jump traction $\Delta\mathbf{t}$ is given by the equation (3). Under these conditions only the integral representation for the fluid-fluid interface S need to be considered, hence

$$\begin{aligned} (1 + \lambda)\mathbf{u}(\mathbf{x}_o) = 2\mathbf{u}^\infty(\mathbf{x}_o) - A \int_S \mathbf{G}(\hat{\mathbf{x}}) \cdot \Delta\mathbf{t}(\mathbf{x}) dS_x + B \int_S \mathbf{u}(\mathbf{x}) \cdot \mathbf{T}(\hat{\mathbf{x}}) \cdot \mathbf{n}(\mathbf{x}) dS_x \\ - A \int_S \mathbf{G}(\hat{\mathbf{x}})(\Delta\rho\mathbf{g} \cdot \mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) dS_x + \frac{(\lambda\Delta' - \Delta)}{2\pi} \int_S r^{-1} \mathbf{n}(\mathbf{x}) dS_x, \end{aligned} \quad (28)$$

where $A = 1/4\pi\mu$ and $B = \frac{3}{2\pi}(\lambda - 1)$.

4. APPLICATIONS OF THE METHOD FOR EMULSION DENSIFICATION

In order to generate realistic high-volume-fraction microstructures, we propose to simulate the centrifugation process by which high-density emulsions are produced from low-density materials (Mason et al. 1997). The extraction of the continuous-phase fluid during this densification process is equivalent to a distributed sink of continuous-phase fluid. Thus, we will simulate this densification process by describing the evolution in a system with a uniformly-distributed sink of continuous-phase fluid.

4.1. Many interacting drops

All simulations rely on the boundary integral method. Periodic boundary conditions are enforced through the use of periodic Green's functions. These are obtained by Ewald summation (Beenker 1986) using accurate computationally-efficient tabulation of the nonsingular background contribution (Loewenberg & Hinch 1996). The appropriate formulation was derived here in §3. The resulting boundary integral formulation are now capable of describing the dynamics of dense emulsions for uniform compressibility. Accordingly, the evolution of M neutrally buoyancy deformable drops is described by time-integrating the fluid velocity $\mathbf{u}(\mathbf{x}_o)$ on a set of interfacial marker points \mathbf{x}_0 on each drop surface. In the present application it is considered the case in which there is a rapid equilibrium of insoluble surfactants (incompressible surfactants). Therefore, marangoni stresses and adsorption-desorption of surfactants can be ignored.

All quantities below are made dimensionless using the (volume-averaged) drop size a and the relaxation rate $\Gamma/\mu a$. The relevant physical parameters that describe the system simulated here: λ , ϕ and the compressibility parameter, $Ca_o = a\mu\Delta/\Gamma$ (ratio of viscous to surface tension stress) is the appropriate capillary number for the densification process. In the absence of an imposed flow (i.e. $\mathbf{u}^\infty(\mathbf{x})_o = \mathbf{0}$), the dimensionless fluid velocity is governed by the second-kind integral equation on the interfaces S_m ($m = 1, \dots, M$) of all drops in the simulation

$$(1 + \lambda)\mathbf{u}(\mathbf{x}_o) - B \sum_{m=1}^M \int_{S_m} \mathbf{u}(\mathbf{x}) \cdot \mathbf{T}^P(\hat{\mathbf{x}}) \cdot \mathbf{n}(\mathbf{x}) dS_x = \mathbf{F}(\mathbf{x}), \quad (29)$$

where

$$\mathbf{F}(\mathbf{x}) = -\frac{1}{4\pi} \sum_{m=1}^M \int_{S_m} \Gamma(\nabla^s \cdot \mathbf{n}) \mathbf{G}^P(\hat{\mathbf{x}}) \cdot \mathbf{n}(\mathbf{x}) dS_x + \frac{Ca_o f(\phi)}{\pi} \sum_{m=1}^M \int_{S_m} \Phi^P(r) \mathbf{n}(\mathbf{x}) dS_x.$$

\mathbf{G}^P and \mathbf{T}^P are respectively the periodic stokeslet and stresslet defined as in Loewenberg & Hinch (1996), Φ^P is the periodically-replicated r^{-1} potential and $f(\phi) = -\Delta [1 + \lambda(\phi^{-1} - 1)]$.

4.2. Description of numerical simulations

Evolution of a drop surface S was simulated by means of a surface discretization with initial number of marker points N_o (Cristini et al. 1998). Marker points are convected with the fluid velocity. During the simulation mesh restructuring is performed on S . After each time step, first marker points are added/subtracted on S as required by condition density function; then global mesh equilibration and reconnection are performed. The surface discretization is equilibrated as a dynamical system of springs. An equilibrium configuration is found by direct numerical simulation of evolution of the system of springs using a second order Runge-Kutta scheme to preserve accurate description of the interface for evaluation of the normal vector \mathbf{n} at each integration step. The iterative process is stable and converges quickly to an equilibrium configuration for a smooth distribution of tractions. The normal vector and curvature were calculated by the local surface-fitting algorithm of Zinchenko et al. (1997). The fluid velocity on the drop interfaces are obtained by an iterative solution of (29) using the GMRES algorithm (a generalization of the conjugate gradient method to non-symmetric matrices) to achieve convergence for the closely-spaced interface configurations that characterize dense emulsions. Once fluid velocity is known, positions of marker points are evolved by a second Runge-Kutta scheme. An appropriate time step that is proportional to the shortest edge length is set to ensure stability.

The adaptive surface triangulation algorithm, described in Cristini et al. (1988), has been extended to construct efficient simulations of dense systems. Accordingly, a new marker point density function was defined that resolves the minimum local length scale everywhere on the drop interfaces. For the proposed problems here the minimum local length scale may depend on the local curvature or local film thickness h . Thus, the marker point density function (??) should be generalized to $\rho_N \sim R_1^{-2} + R_2^{-2} + C_1(|\nabla_s h|/h)^2$, where R_1, R_2 are the local principal radii of curvature, and C_1 are $O(1)$ constants whose precise value is unimportant. The proposed marker point density function resolves the rim of dimpled regions where the film thickness varies rapidly and the lubrication length scale \sqrt{hR} in regions where the film thickness is slowly-varying ($R = \min[R_1, R_2]$). Only rim regions, not flat regions, require high resolution. An inspection of the result in Fig. 1 which was obtained using the new density function, illustrates this point: high resolution is needed on the plateau borders and junctions, not on the flat films between drops. This observation is important for ensuring the feasibility of accurately resolving the dynamics of the closely-spaced interfaces that characterize the dense systems that we have explored.

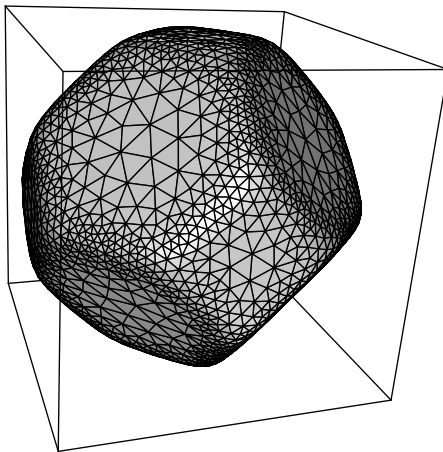


Figure 1: Adaptive grid after a uniform expansion of drops on a BCC lattice evolving into Kelvin cells; $Ca_o = 0.5$ and $\phi = 0.96$, $\lambda = 1.0$.

5. Results of emulsion densification

A wide range of densification processes can be simulated through the appropriate ϕ dependence (i.e., time-dependence) of Δ . It is also possible to explore microstructural manipulation through an applied shear during densification. Here, we consider constant compressibility, quiescent flow conditions and the case $\lambda = 1.0$ because the numerical implementation is simpler. Densification with prescribed nonequilibrium osmotic pressure has been also explored since it corresponds most closely to the experimental procedure that has been developed (Mason et al. 1997). Under these conditions, densification proceeds until the applied osmotic pressure is balanced by the equilibrium osmotic pressure of the emulsion. The simple Kelvin-cell microstructure, depicted in Figs 2, was obtained using our new algorithm based on the compressible formulation discussed in §3. Spherical drops on a BCC lattice make first contact with eight nearest neighbors and form precursors of hexagonal faces when $\phi < \phi_c = \pi 3^{1/2}/8 = 0.68$ (maximum packing for BCC). The results illustrate the evolution of drop shape from spheres to Kelvin cells. Once the emulsion expansion has stopped, the drop shape will continue to relax toward equilibrium; the emulsion expand and then relaxes for twenty time units.

6. Conclusion

The formulation of boundary integral equations for compressible Stokes flow has been discussed. The approach was applied for generating dense compressed emulsion structure in viscous flows with periodic boundary conditions. We have made substantial progress on the problem of emulsion densification. The results demonstrate the feasibility of simulating high-volume-fraction systems. A study of densification may have interesting materials processing applications that will be pursued in a future study.

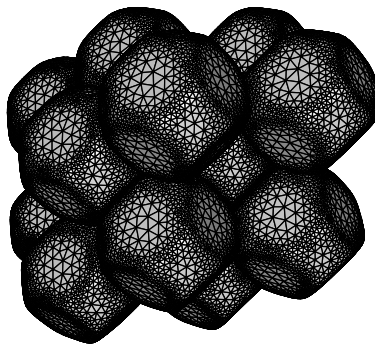


Figure 2: Microstructure of a dense emulsion resulting from expansion of the dispersed-phase with $Ca_o = 0.5$, $\phi = 0.95$ and $\lambda = 1.0$.

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