Viscous flow in domains with corners: Numerical artifacts, their origin and removal

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Abstract

Viscous flows in domains with boundaries forming two-dimensional corners are considered. We examine the case where on each side of the corner the boundary condition for the tangential velocity is formulated in terms of stress. It is shown that computing such flows numerically by straightforwardly applying well-tested algorithms (and numerical codes based on their use, such as COMSOL Multiphysics) can lead to spurious multivaluedness and mesh-dependence in the distribution of the fluid’s pressure. The origin of this difficulty is that, near a corner formed by smooth parts of the boundary, in addition to the solution of the formulated inhomogeneous problem, there also exists an eigensolution. For obtuse corner angles this eigensolution (a) becomes dominant and (b) has a singular radial derivative of velocity at the corner. Despite the bulk pressure in the eigensolution being constant, when the derivatives of the velocity are singular, numerical errors in the velocities calculation near the corner give rise to pressure spikes, whose magnitude increases as the mesh is refined. A method is developed that uses the knowledge about the eigensolution to remove the artifacts in the pressure distribution. The method is first explained in the simple case of a Stokes flow in a corner region and then generalized for the Navier–Stokes equations applied to describe steady and unsteady free-surface flows encountered in problems of dynamic wetting.

1. Introduction

In many problems of computational fluid dynamics, it is necessary to consider domains in which two parts of a piecewise smooth boundary locally form a two-dimensional wedge. An important class of such problems is associated with the modelling of free boundary flows that involve ‘dynamic wetting’ (Fig. 1), that is the process in which a liquid spreads over the surface of a solid. The liquid’s free surface intersects with the surface of the solid at a ‘contact line’ and forms what is referred to as a ‘contact angle’ with it [1,2]. The value of the contact angle can vary, depending on the wetting speed and the overall flow [3–6], so that, to describe the process, one has to be able to solve equations of fluid mechanics in domains where two parts of the boundary locally form wedges of different angles.

It has been known for a long time [7] that classical boundary conditions, when applied in dynamic wetting, i.e. in the situation where the contact line moves with respect to the solid, lead to a physically unacceptable outcome, namely a nonintegrably infinite force acting between the liquid and the solid.¹ Termed the ‘moving contact-line problem’, this difficulty has become the subject of many theoretical works (see Chapter 3 of [6] for a review). The common feature of almost all theoretical models proposed for the moving contact-line problem is that the no-slip boundary condition on the solid surface, i.e. the condition for the tangential component of the fluid’s velocity, is replaced by a more general (slip) condition with all other boundary conditions remaining intact. The case in which the tangential velocity of the fluid on the solid surface is prescribed as an explicit function of distance from the contact line has been considered [9–11]; however, in the overwhelming majority of articles the new boundary condition is formulated for the tangential stress. The most frequently used form of slip (see, for example, [9,10,12,13]), and the only one we shall consider henceforth, is the Navier-slip boundary condition [14] which makes slip, i.e. the difference between the fluid’s velocity and the velocity of the solid, proportional to tangential stress, with a coefficient of proportionality termed ‘the coefficient of sliding friction’ [15].

In most practically relevant situations, the resulting free-boundary problems are untractable analytically and have to be solved numerically. The main difficulty in the numerics of dynamic wetting is the handling of the flow in the immediate vicinity of the contact line, where the obstacles are twofold. Firstly, sufficient grid resolution is required to resolve the small length scales characterizing the flow near the contact line and, secondly, numerical artifacts that could arise due to the non-smooth boundary have to be interpreted and avoided.

¹ In a general case, one has that there is simply no solution that would satisfy all boundary conditions, including the normal-stress condition on the free surface. See [6,8] for detail.

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The first of these difficulties, caused by the region where the no-slip boundary condition is relaxed being extremely small, requires one to ensure that the computational mesh near the corner is sufficiently refined for the slip region to be well resolved. Otherwise, the global effect of the under-resolved corner region could be quite dramatic, as has been emphasized in several recent works \cite{16–18}; this error generation has been quantified in Sprittles and Shikhmurzaev \cite{19} and lies outside the scope of this article in which sufficiently well resolved meshes are always employed. At the same time, away from the contact line, where only bulk length scales need to be resolved, the meshing should not be excessive, for the computations to still be feasible.

The second issue, in the dynamic wetting problem considered, is due to the fact that locally one has a mathematical problem in a wedge region (Fig. 1c), with different boundary conditions on the two sides. Both sets of boundary conditions involve first-order differential operators applied to the tangential component of the bulk velocity and linear homogeneous algebraic conditions for its normal component; that is, on each interface, boundary conditions formulated in terms of the tangential stress and the condition of impermeability. As always, it is important to ensure that the numerical code dealing with such a problem does not give rise to numerical artifacts, which in this case might result from the boundary being not smooth. This is the second and more severe difficulty one faces in numerically solving problems of dynamic wetting, and a necessary condition to ensure the absence of artifacts is that the numerical solution becomes mesh-independent as the mesh size goes down. If this is not the case, there is obviously no convergence of the numerical solution to the one it is supposed to approximate.

It is important to note that if the code gives rise to an artifact, so that the numerical solution is mesh-dependent, then the more one resolves the mesh near the contact line, the more pronounced and unacceptable the artifact becomes. In Sprittles and Shikhmurzaev \cite{20}, the standard finite element method was seen to produce such mesh-dependent oscillatory solutions for the case in which the velocity on the solid is an explicit function of distance from the contact line, as opposed to satisfying the Navier condition. We demonstrated that these numerical issues occurred because the code was attempting to approximate singularities that are inherent in the model and that they may be resolved by using the well-known approach of incorporating specially designed elements adjacent to the corner which allow singular variables to be approximated. One may expect, that the situation we consider in this paper, where the Navier-slip (i.e. Robin-type) condition is applied on the solid surface instead of a Dirichlet condition, would require merely an extension of the methods used in Sprittles and Shikhmurzaev \cite{20}. Intriguingly, we will see that this conjecture is incorrect; the problem considered requires the development of an entirely new computational tool.

In the present work, we show that an attempt to apply well-tested standard numerical methods to the moving contact-line problem in a straightforward way can lead to a numerical artifact which is exacerbated as the mesh is refined. By stripping the moving contact-line problem of ‘additional’ difficulties, we show that even in the simplest case of a steady Stokes flow in a corner region, irrespective of a particular numerical implementation, in a certain range of corner angles the computed bulk pressure is mesh-dependent, as the code attempts to approximate a function which is multivalued at the corner. If the pressure multivaluedness is suppressed using numerical means, then the pressure and velocity fields no longer satisfy the original equations in the bulk. Neither of these options is satisfactory, and the persistent nature of the problem makes it necessary to handle it robustly, beginning by determining its origin.

In order to identify the origin of this behaviour of the numerical solution, we consider an even simpler case of the flow in a wedge formed by zero-tangential-stress boundaries, where an exact analytic solution is available. A comparison of the numerical results with this exact solution, which has a globally constant pressure, shows that the observed ‘multivaluedness’ of pressure is indeed a numerical artifact. Once the zero-tangential-stress boundary condition on one of the boundaries is replaced with the original inhomogeneous Robin-type condition, like the Navier-slip condition, the nature of the artifacts does not change, thus indicating that the artifact is the result of superposition of the spurious solution to the homogeneous (zero-tangential-stress) problem and the solution of the inhomogeneous problem.

The considered cases suggest that the conventional application of the standard numerical methods will lead to numerical artifacts not only in the modelling of dynamic wetting that uses the Navier-slip condition and its generalizations (see, for example, \cite{21,22,6}), but also in many other free-surface flows. Notably, the same type of boundary conditions have been used to model situations in which the contact line is stationary, i.e. it is pinned to the solid at a specific point. This occurs, for example, in the extrusion of a liquid jet from a nozzle \cite{23,24}. We will describe how, for both static and moving contact line problems, the spurious numerical behaviour which we observe has been interpreted as a physical effect in a number of publications. Additionally, we predict that where one has a corner flow with the boundary conditions of the same type, like coalescence of liquid volumes \cite{6} and the cusps/ corners in the free surface generated by convergent flows \cite{25,26}, the same spurious numerical behaviour will appear. The method of removing numerical artifacts developed in the present work applies to all these flows in a straightforward way.

2. Problem formulation

Consider the two-dimensional steady viscous flow of an incompressible Newtonian fluid, with density \( \rho \) and viscosity \( \mu \), in a corner confined by straight boundaries located at \( \theta = 0 \) and \( \theta = \alpha \) of a polar coordinate system \((r,\theta)\) in the plane of flow and the ‘far field’ boundary on an arc of a sufficiently large radius \( r = R \) (Fig. 1c). Conventionally, we will refer to the \( \theta = 0 \) and \( \theta = \alpha \) boundaries as the ‘solid boundary’ and the ‘free surface’, respectively. Finding the free-surface shape, which is planar only to leading order as \( r \to 0 \), is an additional, though rather standard, element of difficulty, not essential to the problem we are going to consider initially. The ‘free surface’ will be made genuinely free, with its shape to be determined, in Section 6.2. Here we are interested in the flow in a corner formed between a prescribed planar free surface and a solid boundary, so that the normal-stress boundary condition, used to find the free surface shape, is not required.

The flow is driven by the motion of a solid at \( \theta = 0 \), which slides with speed \( U \) parallel to itself, and, possibly, also by the far-field conditions. The speed \( U \) will be used as a scale for the fluid’s velocity. For simplicity, we will assume that the velocity and length
scales that characterize the flow are such that the Reynolds number $Re$ based on these scales is small. Then as $Re \to 0$, to leading order in $Re$ we may consider the Stokes flow. It should be emphasized that all essential results remain valid for the full Navier–Stokes equations since they come from the asymptotic behaviour of the solution as $r \to 0$. Considering the Stokes flow allows us to demonstrate the method we use to handle the pressure multivaluedness more clearly, without additional but nonessential details associated with handling nonlinear convective terms. These details are described in Section 6.2.

For the problem in question, the non-dimensional Stokes equations for the bulk pressure $p$ and the radial and azimuthal components of velocity $(u,v)$ take the form

$$
\frac{1}{r} \frac{\partial (ru)}{\partial r} + \frac{1}{r} \frac{\partial v}{\partial \theta} = 0 \quad (0 < r < R, 0 < \theta < \pi),
$$

(1)

$$
\frac{\partial p}{\partial r} = A u - \frac{u}{r^2} - 2 \frac{\partial u}{\partial r}, \quad \frac{1}{r} \frac{\partial v}{\partial \theta} = A v - \frac{v}{r^2} - 2 \frac{\partial v}{\partial r},
$$

(2a,b)

where

$$
A = \frac{\partial^2}{\partial \theta^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2}.
$$

On the solid surface, for a solution not to have a multivalued velocity at the corner [6,27], we use the Navier slip condition [14], as opposed to the no-slip condition of classical fluid mechanics, and keep intact the impermeability condition for the normal component of velocity to the surface:

$$
\frac{\partial u}{\partial r} = \bar{t} \hat{v}(u - 1), \quad v = 0 \quad (0 < r < R, \theta = 0).
$$

(3a,b)

Here $\bar{t}$ is the dimensionless ‘coefficient of sliding friction’ [15]. In the limits $\beta \to 0$ and $\beta \to \infty$, one recovers the conditions of zero tangential stress (free slip) and no-slip, respectively. The value of $1/\beta$ is proportional to a (non-dimensional) ‘slip length’ that characterizes the region where the velocity field specified with the help of the Navier condition (3a,b) deviates from the velocity field which would have been specified by no-slip.

On the free surface, we have the standard boundary conditions of zero tangential stress and impermeability:

$$
\frac{\partial u}{\partial \theta} = 0, \quad v = 0 \quad (0 < r < R, \theta = \pi).
$$

(4a,b)

The boundary conditions in the far field can be imposed in different ways. For simplicity, we will make the far-field conditions ‘passive’ and assume that

$$
\frac{\partial u}{\partial r} - \frac{\partial v}{\partial \theta} = 0 \quad (r = R, 0 < \theta < \pi).
$$

(5)

This condition is an adaptation for a finite domain of a boundary condition that would specify the asymptotic behaviour of the flow field at infinity. As is known [28], this condition is satisfied if the Navier slip condition (3a) is replaced by no-slip (i.e. for $\beta = \infty$ in (3a)), so that (5) can be seen as a condition that the disturbance caused by finiteness of $\bar{t}$ attenuates in the far field. In computations, for the far-field to have a negligible effect on the near-field flow, it is sufficient to put $R \gg 100/\beta$.

Eqs. (1)–(5) fully specify the problem of interest.

3. Local asymptotics

The defining feature of our problem is the angle formed by two parts of the boundary and, for future references, it is useful to reproduce the leading-order asymptotics for the solution of (1)–(5) as $r \to 0$ [6,8]. After introducing the stream function $\psi$ by

$$
u = \frac{1}{r} \frac{\partial \psi}{\partial r}, \quad v = \frac{\partial \psi}{\partial \theta}, \quad (6a,b)
$$

Eqs. (1) and (2a,b) are reduced to a biharmonic equation $A^2 \psi = 0$ with boundary conditions (3a,b) and (4a,b) taking the form

$$
\frac{\partial^2 \psi}{\partial r^2} - \frac{\bar{t} \hat{v}}{r} \left( \frac{\partial \psi}{\partial \theta} - r \right), \quad \psi = 0 \quad (0 = \theta = 0, 0 < r < R),
$$

(7a)

$$
\frac{\partial^2 \psi}{\partial \theta^2} = 0, \quad \psi = 0 \quad (\theta = \pi, 0 < r < R).
$$

(8a,b)

Condition (7a), which is the only inhomogeneous boundary condition in the problem (i.e. the condition that drives the flow), suggests looking for the leading-order term of the local asymptotics in the form $\psi = r^2 F(\theta)$, which is one of a family of separable solutions to the biharmonic equation of the form $\psi = r^2 F(\theta)$. After substituting $\psi$ into the biharmonic equation and boundary conditions (7a,b) and (8a,b), we have that

$$
\psi = r^2 (B_1 + B_2 \theta + B_3 \sin 2\theta + B_4 \cos 2\theta),
$$

(9)

where the constants of integration $B_i (i = 1, \ldots, 4)$ are: $B_1 = -B_5 = -\beta/4, B_2 = -B_1/2, B_3 = B_5 \cot 2\theta$.

The pressure field obtained from (2) using (6) and (9) has the form

$$
p = \frac{\tilde{p}}{2} \ln r + p_0,
$$

(10)

where $p_0$ is a constant which sets the pressure level.

The derived local solution to the full inhomogeneous problem (9) and (10) could be superimposed with an eigensolution, i.e. a solution satisfying homogeneous boundary conditions, $v = \partial u/\partial \theta = 0 (0 = \theta = \pi)$. An eigensolution to our problem has been known for a long time [28, p. 14] and is known to be important for determining the flow past a static contact line [24,29]. In terms of the stream function, it also has a separable form:

$$
\psi_c = Ar^2 \sin (\lambda \theta), \quad \lambda = \pi/\alpha,
$$

(11)

where $A$ is an arbitrary constant.

Surprisingly, the eigensolution (11) produces a $\textit{globally constant}$ pressure, so that the leading order pressure is always determined from (10), which is logarithmically singular at the corner. Notably, the pressure never depends on the angular coordinate $\theta$.

The eigensolution’s velocity distribution is not trivial and, by comparing (9) and (11), one can see that for $\lambda < 2$, i.e. $\alpha > \pi/2$, it will dominate the solution to the inhomogeneous problem (9). The transition between different flow regimes will occur at $\alpha = \pi/2$, with the eigensolution becoming dominant above this value, i.e. for obtuse angles. This means that for acute angles, as $r \to 0$, the velocity scales linearly with $r$ whilst for obtuse ones the velocity has asymptotic behaviour $r^{2-\lambda}$ so that, in the aforementioned limit, the radial derivative of velocity will be singular. Interestingly, for acute angles the leading order asymptotic solution may be fully derived, whilst for obtuse angles the eigensolution, which dominates the flow, is pre-multiplied by an undetermined constant $A$. Consequently, for obtuse angles the leading order asymptotics provides a whole one-parametric family of solutions, so that a quantitative comparison of the velocity obtained from our numerical code and the asymptotic result is no longer possible. However, the eigensolution creates a globally constant pressure so that for obtuse angles we are still able to compare the pressure obtained numerically with the asymptotic solution at the same level of accuracy as for acute angles, i.e. up to an additive constant.

We should require that the performance of our code is not influenced by the characteristic behaviour of the flow as the corner is approached. To ensure this standard is achieved, we use our code to simulate flow at both acute and obtuse angles, beginning with the former.
4. Numerical results

The problem formulated in the previous section was solved using a pre-existing numerical code based on the Galerkin finite element method. The main elements of the code are described in the Appendix for the case of the unsteady dynamic wetting problem considered in Section 6.2: flow in a wedge shaped domain is just a special, simple, case of this implementation. A user-friendly step-by-step guide specifying the entire implementation can be found in Sprittles and Shikhmurzaev [19]. The same code has previously been used to simulate the flow of liquids over chemically patterned surfaces [30,31], where it was shown how the effect of variable wettability of the solid surface on the flow of an adjacent fluid can be described in the framework of continuum mechanics, in agreement with the results of molecular dynamics simulations [32,33].

Convergence of our computational solutions as the spatial resolution of the mesh is increased has been established in Sprittles and Shikhmurzaev [19], where the mesh resolution required to attain a predicted accuracy in the numerical solution is determined in terms of the non-dimensional similarity parameters appearing in dynamic wetting problem. This issue is outside the scope of this paper and curves from any mesh independent results presented in the forthcoming sections of this article are graphically indistinguishable from those obtained with further mesh refinement.

As an additional test of the robustness of our numerical results and the ubiquity of the emerging numerical artifacts (described below) for the flows in the corner regions that we are examining here, these results have been verified for test cases using a commercially available code, COMSOL Multiphysics. All computations presented below correspond to \( \beta = 10 \), \( R = 10 \); the runs in the process of investigation covered a wide range of parameters to ensure that the features described below are invariant with respect to variations of these parameters.

4.1. Acute wedge angles

First, we consider the case of \( \alpha < \pi/2 \) where the eigensolution does not influence the leading order behaviour of either the velocity or the pressure. Our numerical results will be shown to be in excellent agreement with the local asymptotics described earlier.

The streamlines in Fig. 2 illustrate the general features of the flow: motion is created by the relative movement of the solid surface with respect to the corner, and the fluid near the solid is pulled out of the corner by the moving substrate and, by continuity, it is replenished there by an inflow from the far field.

The pressure distribution near the corner in the form of isobars and, to make it easier to envisage, a 3-dimensional plot are shown in Fig. 3. As predicted by Eq. (10) of the local asymptotics, which is the leading order solution for all angles, the pressure in the vicinity of the corner is independent of \( \theta \).

The quantitative comparison of the computed velocity and pressure with those given by the asymptotics is shown in Fig. 4. As one can see, the agreement between numerical and analytic results for the distribution of velocity and pressure is excellent. The velocity is linear whilst the pressure, which is plotted in a semi-logarithmic frame, is logarithmic with the expected gradient. The pressure constant \( p_0 \) in (10) has been chosen to provide the best fit, but does not in any way determine the shape or gradient of the curve.

4.2. Obtuse angles: multivaluedness of pressure

In the previous subsection, we have shown that our algorithm gives excellent results for \( \alpha < \pi/2 \). However, for the angles \( \alpha > \pi/2 \) the situation changes. The same code, as well as COMSOL Multiphysics, that we used for comparison, produces results that are markedly mesh-dependent. This means that, at least, the numerical solution cannot be regarded as a uniformly valid approximation of the exact one, and, possibly, that it is completely spurious.

Fig. 5 shows the picture of streamlines near the corner. The dominance of the eigensolution in the near field ensures that the flow is faster than that obtained for acute angles. There is no indication of any particular abnormality, at least on a qualitative level. Interestingly, once the angle becomes obtuse, the inhomogeneous asymptotic solution (9) predicts that near the corner the flow along the free surface is in the upstream direction, i.e. the radial component of velocity along the free surface is positive. It is the presence of the eigensolution, which becomes dominant for obtuse angles, that ensures a regular downstream flow with the velocity on the free surface directed towards the corner, as one may intuitively expect. The behaviour is confirmed in Fig. 6, where one can observe that the numerically computed velocity distribution differs considerably from the asymptotic solution to the inhomogeneous problem, which predicts flow reversal, most noticeably no longer behaving linearly with radius. So far, the numerical solution has been shown to be in excellent quantitative agreement with the asymptotic one for acute angles, and the velocity distribution at obtuse angles has the expected form.

To ensure quantitative agreement between the asymptotic and numerical solutions for obtuse angles, we recall that the pressure contribution from the eigensolution has no impact on the leading order asymptotic solution. Therefore, we should expect the pressure to have the same behaviour as observed for acute angles. However, when we examine the plots of the pressure distribution near the corner shown in Fig. 7, it becomes immediately clear that there are severe numerical issues. The smooth \( \theta \)-independent pressure obtained for acute angles is now replaced by two huge spikes of differing signs at the nodes adjacent to the corner. The more we refine the mesh, the larger the spikes become. The distribution of pressure along the boundaries near the corner shown in Fig. 6 confirms that we have a problem to resolve. The numerical method implies single-valuedness for both velocity components and the pressure at the corner, and computations confirm single-valuedness of velocity 2 (Fig. 6).

The situation with the pressure is severe. As one can see from Figs. 6 and 7, the numerical scheme is attempting to approximate a function which is both singular and multivalued at the corner. As one approaches the corner along different radii, the pressure behaves differently and tends to plus infinity along the radii closer

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Fig. 2. Streamlines for \( \alpha = \pi/4 \) in increments of \( \psi = 0.02 \) with the boundaries at \( \theta = 0 \) and at \( \theta = \pi \) corresponding to \( \psi = 0 \).

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2 Its single-valuedness is ensured by the slip boundary condition [1,27], whereas, numerically, once we assume all functions to be single-valued, the impermeability conditions make the corner a stagnation point.
to the free surface and to minus infinity along those closer to the solid boundary. Since the numerical scheme imposes (artificial) single-valuedness at the corner by stating that pressure has one value at the corner node, the code tries to reconcile the calculated pressure with this requirement over the first row of elements, thus creating the cliffs shown in Fig. 7. The numerical results are mesh-dependent: the smaller one makes the size of the first row of elements, the nearer the multivalued solution approaches the corner, and the higher the cliffs of pressure become. Obviously, the mesh-dependent numerical results cannot be regarded as a uniformly valid approximation of the actual solution to (1)–(5) and hence have to be rejected. As shown by the semi-logarithmic plot in Fig. 6, the singularity of pressure at the corner is also stronger than

Fig. 3. Pressure distributions in the vicinity of the corner for $\phi = \pi/4$. Left: pressure contours in steps of size 5, as the corner is approached with the underlying finite element mesh visible. Right: surface plot of pressure.

Fig. 4. Left: comparison of the computed radial velocity $u$ along the liquid–solid interface 1 and liquid–gas interface 2 with the corresponding asymptotic solution to the inhomogeneous problem 1A and 2A, respectively. Right: comparison of the computed pressure along the interfaces to the asymptotic result (dashed line).

Fig. 5. Streamlines for $\phi = 3\pi/4$ in increments of $\psi = 0.04$ with the boundaries at $\theta = 0$ and at $\theta = \phi$ corresponding to $\psi = 0$.

Fig. 6. Left: comparison of the computed radial velocity $u$ along the liquid–solid interface 1 and liquid–gas interface 2 with the asymptotic solution to the inhomogeneous problem 1A and 2A (i.e. without the eigensolution’s unknown contribution), respectively. Right: computed pressure along the interfaces.

Fig. 7. Pressure distributions in the vicinity of the corner for $\phi = 3\pi/4$. Left: pressure contours as the corner is approached with the underlying finite element mesh visible. Right: surface plot of pressure.
logarithmic (by plotting the pressure in the log–log frame one can show that it is actually algebraic with the exponent dependent on $\alpha$).

It should be emphasized that the difficulties we are describing are above the level of a particular numerical implementation of a particular algorithm. It is not only that the code we used has been thoroughly validated (see the previous section); additionally, the commercially available code COMSOL Multiphysics has also been applied to the wedge flow problem for both acute and obtuse angles, and in all cases identical results have been recorded.

4.3. Remedies described in the literature

The encountered problem is resilient to standard approaches which have been described in the literature as successful remedies to spurious numerical effects. The first approach to be tried is to incorporate the asymptotic results described earlier in the numerical scheme to ‘come out’ of the corner, thus bypassing any spurious effects that might have been caused by the geometry. The asymptotics can be matched with the numerical solution outside a given radius in a variety of ways. This approach has proved successful in similar situations in which corner singularities exist [34]. However, it has been found that for our problem such an alteration of the scheme merely shifts the pressure cliff to the arc at the radius where the asymptotics has been applied. This is of no help whatsoever, since the results have all the deficiencies listed above.

The singular element method, used in Sprittles and Shikhmurzaev [20], falls into the aforementioned class of remedies. This method works when the computed solution closely approximates the asymptotic result in all but a small region near the corner where a singularity is present and hence a code with finite elements can then be generated only by the boundary conditions in the far field. Incorporating singular elements allows the pressure at the corner to be ‘tied-up’, using the asymptotic form of the solution, and in Sprittles and Shikhmurzaev [20] the method was generalized to account for the influence of eigensolutions with singular pressure behaviour. However, in the present work, the eigensolution derived in Section 3 is not singular and, contrary to what the asymptotics predicts, the code clearly tries to approximate a function that is not only singular but also multivalued at the corner. Therefore, singular elements based on the (single-valued) asymptotic solution are bound to fail to address this issue. As our test runs have confirmed, the method of singular elements indeed fails to remove the spurious pressure behaviour.

Another standard approach is to impose penalties of various forms, similar to those used with equal-order interpolation to circumvent the LBB condition [35], but such a method simply fails to drive the code into a mesh-independent solution. The extent to which the penalties flatten the pressure cliffs is exactly the extent to which the numerical solution (to the ‘penalized problem’) departs from that which would satisfy the original problem discretized using the standard FEM. In other words, instead of driving the code to the ‘right’ solution, the penalty becomes part of the differential equations the code is solving, i.e. the method effectively replaces the original problem with a different one.

The pressure behaviour which we have described has previously been observed, suspected of being spurious and designated as the subject of future research in a paper on the finite element simulation of curtain coating [36]. As is pointed out in this paper, a reason that the problem may have not been treated in other investigations is a lack of computational resolution. A rough indication of the region which must be resolved by any numerical scheme is the slip length, given by $1/\beta$. Tests show that at least 100 nodes should be used along each radial-ray within this region. With the graded mesh we have used and for modern computers this requirement causes no problem. For a mesh with a single element size, achieving this is more difficult, as the numerical cost of having every element of size $0.01/\beta$ could render the computational task untractable. It may be that this is the case in a number of older publications in which computational power proved a major problem [37, 38]. In our calculations presented here, the smallest element has the size of $4 \times 10^{-3}$, and we have 206 nodes inside the slip length along each radial-ray.

5. Origin of the pressure multivaluedness: a model situation with an analytic solution

The numerical difficulties we have encountered occur when the eigensolution should be the dominant feature of the near field flow. Note that, although the velocity of the eigensolution tends to zero at the corner, its radial dependence scales like $r^{-1}$, and hence for $\pi/2 < \alpha < \pi$ the derivatives of velocity in the radial direction are singular at the corner. Consequently, the computed pressure behaviour could result from numerical errors in calculating the velocity field corresponding to this eigensolution.

As previously noted, the eigensolution (11) produces a globally constant pressure. This simplicity allows an ideal opportunity to check whether the spikes associated with the multivaluedness of pressure computed earlier are indeed numerical artifacts. In order to do this, we consider the flow in a corner region with the Navier slip condition replaced with zero tangential stress, i.e. with $\partial u/\partial \theta = 0$ and $v = 0$ on both boundaries $\theta = 0$ and $\theta = \alpha$. The flow can then be generated only by the boundary conditions in the far field which we set using the eigensolution (11), where, for simplicity, we use $A = 1/\lambda$:  
\[
\begin{align*}
  u &= r^{-1} \cos(\lambda \theta), \\
  v &= -r^{\lambda-1} \sin(\lambda \theta) \\
  \quad (r = R, \ 0 < \theta < \alpha).
\end{align*}
\]

Then the eigensolution is the exact global solution to our test problem. As for the pressure distribution, once the pressure level has been set, say, to zero, then one will have $p = 0$ in the whole domain. Once this problem is computed numerically, the situation becomes clear. Fig. 8 shows the isobars and a 3-dimensional plot obtained using our code. The isobars and the 3-dimensional plot resemble those which we have already seen for the Navier condition in the previous section, with the same cliffs in the pressure profile at the nodes nearest to the corner. This is a remarkable result given that we know the global solution is in fact $p \equiv 0$! Thus, we may now conclude that the pressure cliffs are spurious and have a numerical origin.

![Fig. 8. Pressure distributions in the vicinity of the corner for $\alpha = 3\pi/4$ using our numerical code. The underlying finite element mesh is visible in both plots. Left: pressure contours as the corner is approached. Right: surface plot of pressure.](image-url)
5.1. Persistence of the problem

Exactly the same computational problem was solved using COMSOL Multiphysics. Here, the condition of impermeability and zero tangential stress is selected as a boundary condition by choosing boundary ‘wall’ and then choosing the type ‘slip’. Once again, the V6P3 element is used, but now the mesh, visible for both plots in Fig. 9, has been generated by COMSOL using adaptive grid refinement techniques, and it is unstructured. At the end of the refinement procedure the mesh had 24,343 elements and convergence was achieved when all of the residuals fell below $10^{-12}$.

Fig. 9 shows the isobars and a 3-dimensional plot obtained using COMSOL Multiphysics. These results are in perfect quantitative agreement in the far field with what was obtained using our code and are seen to be similar in the near field (compare to Fig. 8); there is little point in comparing specific values in the near field as the results are seen to be mesh dependent for both codes.

The same spurious features of the numerical solution have been encountered for both the unstructured mesh of COMSOL and the structured mesh of our numerical code, thus suggesting that any alternative mesh design would not allow a route out of the problem. Additionally, COMSOL offers the choice of ten different elements, and, as we have tested, the choice of any of these elements does not affect the overall picture.

The conclusion we have arrived at is important: the spurious pressure spikes we described above have been reported in the literature and a number of incorrect conclusions have been reached. When an angle formed with the solid surface by the contact line, so that the computed normal stress field is actually multivalued, we can subtract this solution from the problem and use the degree of freedom it offers, i.e. arbitrariness of $A$ in (11), to ensure single-valuedness of pressure at the corner. Once the supplementary (to the eigensolution) velocity and pressure fields are computed, we can put the eigensolution, i.e. the velocity field described by (11) and uniformly zero pressure, back. The resulting solution will have the analytically known eigencomponent of the velocity field superimposed on the numerically computed ‘supplementary’ flow and single-valued pressure, and it will satisfy the original equations and boundary conditions.

6. Removal of pressure multivaluedness

First, we will describe the method of removing the pressure multivaluedness from the numerical solution of the problem formulated in Section 2, i.e. for the Stokes flow in a wedge region, and then show how the method can be ‘localized’ to apply to general 2-dimensional Navier–Stokes flows, both steady and unsteady, where an angle formed with the solid surface by a priori unknown free boundaries is but one element.

The key idea of the method is very simple. In the situation where, as in our case, the eigensolution is the cause of the pressure multivaluedness, we can subtract this solution from the problem and use the degree of freedom it offers, i.e. arbitrariness of $A$ in (11), to ensure single-valuedness of pressure at the corner. Once the supplementary (to the eigensolution) velocity and pressure fields are computed, we can put the eigensolution, i.e. the velocity field described by (11) and uniformly zero pressure, back. The resulting solution will have the analytically known eigencomponent of the velocity field superimposed on the numerically computed ‘supplementary’ flow and single-valued pressure, and it will satisfy the original equations and boundary conditions.

6.1. Simplest case: Stokes flow in a corner region

For the problem formulated in Section 2, consider the velocity and pressure as sums of the eigensolution:

$$u_e = A \lambda \bar{r}^{-1} \cos (\lambda \bar{r}), \quad v_e = -A \lambda \bar{r}^{-1} \sin (\lambda \bar{r}), \quad p_e = 0 \quad (\lambda = \pi/x), \quad (13a, b, c)$$

and the components to be computed (hereafter these are marked with a tilde):

$$\langle \tilde{u}, \tilde{v}, \tilde{p} \rangle = \langle u, v, p \rangle + \langle \tilde{u}, \tilde{v}, \tilde{p} \rangle. \quad (14)$$

The constant $A$ in (13a,b) is yet to be specified.

Since the eigensolution satisfies the Stokes equations (1)–(2) and the free surface boundary conditions (4a,b) exactly, one has that $\tilde{u}, \tilde{v}$ and $\tilde{p}$ have to satisfy the unaltered Stokes Eqs. (1)–(2) and boundary conditions (4), whereas the boundary conditions on the solid surface and in the far field for these variables will take the form

$$\frac{\partial \tilde{u}}{\partial \bar{r}} = r \tilde{p}(A \lambda \bar{r}^{-1} + \tilde{u} - 1), \quad \tilde{v} = 0 \quad (0 < \bar{r} < R, \ \theta = 0), \quad (15a, b)$$

$$\frac{\partial \tilde{u}}{\partial \bar{r}} = -A \lambda (\lambda - 1) \bar{r} r^{-2} \cos (\lambda \bar{r}), \quad \tilde{p} = A \lambda (\lambda - 1) \bar{r} r^{-2} \sin (\lambda \bar{r}) \quad (r = R, \ 0 < \theta < x). \quad (16a, b)$$

To complete the problem formulation for $\tilde{u}, \tilde{v}$ and $\tilde{p}$, we must add an equation to account for the additional unknown constant $A$. To do so, we impose a condition that the pressure is single valued at the corner:

$$\lim_{r \to 0} \frac{\partial \tilde{p}}{\partial \bar{r}} = 0. \quad (17)$$

Qualitatively, this condition can be explained as follows. The method is based on taking the eigensolution out of the total and hence ensuring that $\langle \tilde{u}, \tilde{v} \rangle$ do not have the singularity of the radial...
derivatives at the corner, and the numerical error in their computation will not give rise to the errors in computations of the pressure which result in its multivaluedness. By imposing (17), we are effectively ensuring that the eigensolution is taken out fully from the viewpoint of what this subtraction is aimed at achieving. In other words, out of a one-parametric family of eigensolutions, parameterised by the constant $A$, condition (17) selects the one that underpins the flow we are considering.

A simple way for us to impose (17) numerically is to demand that the pressures at the nodes nearest to the corner on the free surface and on the solid boundary are equal, as in our mesh they are equidistant from the corner.

Eqs. (1), (2), (4) and (15)–(17) have been solved using our numerical code with the same solution procedure as before. The streamlines of the supplementary flow obtained from the computation are shown in Fig. 10 alongside the streamlines to our original problem formulated in Section 2, obtained using (14). Although the underlying asymptotic solution predicts that there must be flow reversal near the corner, which is replicated in our numerical solution for $(\bar{u}, \bar{v})$, this feature is blown away by the strength of the eigensolution when it is superimposed on top.

The pressure plots in Fig. 11 show a qualitative transformation from those observed in previous sections: the pressure is now single valued, smooth and exhibits no mesh-dependence. Both the isobars and the 3D surface plot are now similar to those obtained earlier for acute angles (Fig. 3).

The comparison with the asymptotics of Section 3 is shown in Figs. 12 and 13. The agreement of pressure is visibly excellent. One can also observe that the radial velocity along the interfaces $\bar{u}$ and its asymptotic prediction only coincide in a much smaller region than previously observed for acute angles. This is no surprise, given that the eigensolution now enters the Navier condition (15a), where the first term in brackets on the right-hand side becomes small compared to the last term only very close to the corner.

Interestingly, the dominance of the eigensolution in the combined solution for obtuse angles ensures that the velocity field near the corner is almost anti-symmetric about the centre line $\theta = a/2$, whereas for acute angles this is not the case.

Thus, for the present problem of flow in a corner, we have fully resolved the situation. However, when considering more complicated flows, which involve a corner only as an element, the method of removing the eigensolution from the problem formulation throughout the entire domain could become unnecessarily complicated; the eigensolution is only important near one corner and yet it will make artificial contributions to equations and boundary conditions in the whole domain. A more reasonable approach would be to design a ‘local’ variant of the method to remove the eigensolution only near the corner, where its presence creates the unwanted numerical artifacts, leaving the rest of the flow domain intact. This variant of the method is considered below.
6.2. General case: Navier–Stokes equations in domains with curvilinear free boundaries

We will begin by describing the pressure regularization method in its generic form and then illustrate it by considering two test problems: (a) a steady propagation of a meniscus in a channel with plane-parallel walls (Fig. 1a) and (b) an unsteady spreading of a (2-dimensional) liquid drop over a solid surface (Fig. 1b). Now, we have that the bulk flow is described by the full Navier–Stokes equations up to the corner (which, in accordance with the literature, we will now call the ‘contact line’) and the position of the curved free surface is a priori unknown.

After non-dimensionalizing the problem using characteristic length $L$ and velocity $U$ scales from the global flow the incompressible Navier–Stokes equations in the bulk are

$$\nabla \cdot \mathbf{u} = 0, \quad \text{Re} \left[\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} + \frac{\nabla p}{\rho} + \mathbf{St} \mathbf{g}\right] = \nabla \cdot \mathbf{T}.$$

Thus, after decomposing the solution in the inner region into the sum of the eigensolution and the supplementary part to be computed,

$$\mathbf{u}(p) = \left(\mathbf{u}_{\text{in}}, 0\right) + \left(\mathbf{u}_{\text{out}}, p\right),$$

in the inner region we need to:

(i) Take into account the contribution of the eigensolution to the bulk equations ((18a)–(c)) for $\mathbf{u}$ and $p$ arising from the fact that the eigensolution satisfies the Stokes equations, i.e. $\nabla \cdot \mathbf{u}_e = \nabla \cdot \mathbf{P}_e = 0$, where

$$\mathbf{P}_e = \left[\nabla \mathbf{u}_e + \left(\nabla \mathbf{u}_e\right)^T\right]$$

is the stress tensor of the eigensolution, but not the Navier–Stokes equations. Then we have:

$$\nabla \cdot \mathbf{u} = 0, \quad \text{Re} \left[\frac{\partial \left(\mathbf{u} + \mathbf{u}_e\right)}{\partial t} + (\mathbf{u} + \mathbf{u}_e) \cdot \nabla (\mathbf{u} + \mathbf{u}_e)\right] = \nabla \cdot \mathbf{P} + \mathbf{St} \mathbf{g}.$$  

(ii) Take into account, as we did in Section 6.1, the contribution of the eigensolution to the boundary conditions (19) for $\mathbf{u}$ on the solid surface:

$$\mathbf{n} \cdot \mathbf{P} \cdot (I - \mathbf{nn}) = \mathbf{P}_e \cdot (I - \mathbf{nn}),$$

$$\left(\mathbf{u} + \mathbf{u}_e - \mathbf{U}_w\right) \cdot \mathbf{n} = 0.$$  

(iii) Take into account the contribution of the eigensolution to the boundary conditions for $\mathbf{u}$ and $p$ on the free surface (20) that appears due to the fact that now the free surface, being genuinely free, is not necessarily planar, so that

$$\text{Con} \cdot \left(\mathbf{P} + \mathbf{P}_e\right) = \mathbf{n} \nabla \cdot \mathbf{n} \cdot \left(\frac{\partial f}{\partial t} + (\mathbf{u} + \mathbf{u}_e) \cdot \nabla f\right) = 0.$$  

(iv) Formulate the matching conditions at the internal boundary that would link $\mathbf{u}$ and $p$ with the outer flow. These conditions are necessary to calculate solutions in both the inner region and the outer region; these calculations are carried out simultaneously. At the internal boundary, we enforce continuity on the velocity and the stress:

$$\mathbf{u}_o + \mathbf{u} = \mathbf{u}_{\text{out}}, \quad \mathbf{n} \cdot (\mathbf{P}_o + \mathbf{P}) = \mathbf{n} \cdot P_{\text{out}}.$$  

where $\mathbf{n}$ is a normal to the internal boundary and the subscript $\text{out}$ marks the velocity and stress in the outer region that also have to be computed.
In the numerical implementation, care must be taken in the evaluation of the term \( \mathbf{n} \cdot \mathbf{P} \) in (27a) as, although integrable, it is singular in the limit \( r \to 0 \). The term is best evaluated by calculating the stress tensor analytically, rather than using the finite element approximation, or whatever other discretization has been chosen, for the derivatives of the eigensolution’s velocity components in (24).

An internal boundary separating the inner region from the outer flow should lie sufficiently far away from the contact line for the eigensolution to be well within the inner region and at the same time not too far for the regularization method to be localized, as opposed to applied to an unnecessarily large region of the overall flow. Another consideration is how the position of the internal boundary correlates with the computational mesh. In our numerical method this is most easily achieved by using one of the arcs formed by the edges of the finite elements; the method is equally applicable for an algorithm with an unstructured mesh, though the ease of defining the internal boundary will be lost.

Conditions of continuity on the actual solution (28a,b) can be applied in any numerical scheme, but are especially simple to implement in the finite element method where the continuity of stress across a boundary is naturally accounted for.

In order to illustrate how the method works, we consider a pair of two-dimensional test problems (the moving meniscus and the spreading drop) using a Cartesian frame \( \mathbf{x} = (x,y) \) with a solid surface at \( y = 0 \). In our simulations, we fix the parameters to \( Ca = 0.1, Re = 1 \), \( \beta = 10 \) whilst \( St = 0 \) for the propagating meniscus and \( St = 1 \) for the drop spreading. As our interest here lies in the numerical approximation of these flows, as opposed to a detailed comparison with experiment, we may consider, for simplicity, the dynamic contact angle to have a fixed value of \( \alpha = 3\pi/4 \).

The first test problem is the steady motion of a meniscus that a liquid–gas interface forms between plane-parallel walls. In a frame moving with the contact line, the problem is time-independent and hence the time derivatives in both the inner and outer region are zero. The velocity of the solid substrate in the moving reference frame is \( \mathbf{U}_w = (1,0) \).

Fig. 14 shows the velocity fields as they have been computed and the resulting (combined) velocity field. In the top picture, we can see the outer flow and a much weaker supplementary flow in the inner region. When the eigensolution is superimposed back on top of the supplementary velocity field in the inner region, the streamlines are seen to not feel the presence of the internal boundary – the matching conditions work perfectly leaving no ‘scar’ on the flow. As one can observe, peculiarities of the underlying (supplementary) flow in the inner region, such as flow reversal, are of little consequence as their effect is negligible compared to that of the eigensolution. In the plots of pressure in this figure, we show both the pressure using our transition region, demonstrating no ‘scar’ on the pressure field, and additionally, to demonstrate the effect of our method, show the pressure computed for this problem without using our special approach.

Finally, we show that our method is equally applicable to time-dependent flows. As an illustration, we consider the spreading of a two-dimensional liquid drop over the solid surface which is driven from its initially cylindrical shape by gravity. In Fig. 15, we show a snapshot of the streamlines near the contact line in a frame moving...
with the contact line. The free surface is in a state of evolution and hence no longer represents a streamline. Again, a comparison of the two plots in the figure show that the position of the transition line does not affect the overall flow.

7. Conclusion

We have shown that straightforward application of a standard numerical method to a seemingly ordinary fluid-mechanical problem can lead to unacceptable and very persistent numerical artifacts, despite the fact that the conventional preliminary asymptotic analysis of possible sources of difficulties (in our case, the corner formed by smooth parts of the domain’s boundary and a discontinuity in the boundary conditions) does not flag up any concerns. Previous remedies used to resolve numerical problems that occur due to the singular behaviour of variables as the corner is approached, such as the singular element method and various regularization techniques, are shown to be completely inadequate in this case. The errors generated by the spurious pressure behaviour are far from just being confined to the corner: they affect the solution in a significant portion of the computational domain.

A surprising result from the present study is that errors in approximating the velocity field manifest themselves as spurious behaviour in the pressure field. This artifact could remain hidden if the spatial resolution of the code in the potentially problematic region is too low, but it will inevitably manifest itself in the mesh-dependence of the numerical results once the spatial resolution is increased. As we have shown, it is the presence of an underlying eigensolution that creates these numerical artifacts in the pressure distribution, despite the fact that the eigensolution itself has a globally constant pressure.

If the eigensolution is not removed prior to computations, one invariably ends up with huge pressure spikes whose position and magnitude are both mesh-dependent. The numerical analysis indicates that the cause of this numerical instability is the errors in approximating the velocity gradient, as in the eigensolution this gradient is singular at the corner.

The ‘mechanism’ of this error generation could be the subject of a pure mathematical investigation, which could determine general conditions when cross-effects between the velocity and pressure lead to artifacts in the behaviour of one of these parameters in the numerical computations. This exciting new direction of research lies outside the scope of the present paper.

The developed method of removing numerical artifacts in the pressure distribution is not only successful with respect to the model case of a steady two-dimensional Stokes flow in a corner region, but, as is shown, it admits a straightforward generalization which makes it applicable to a general case of unsteady free-boundary Navier–Stokes flow. In practical applications to problems of dynamic wetting one often has a situation where in the process of computations the contact angle varies in a wide range, from the angles where a standard numerical code produces no artifacts to those where the pressure spikes and multivaluedness invariably appear. General-purpose numerical algorithms should be developed so that the present method is turned off for acute angles, where the pressure is naturally single-valued, and switched on for obtuse angles to suppress spurious numerical behaviour.

The issues encountered in this paper will undoubtedly also arise in fully three-dimensional simulations where, in the simplest case, the flow near the contact line can be considered as the superposition of a two-dimensional flow, as considered in this paper, with a correction caused by the cross-flow tangential to the contact line. The techniques developed in this paper are easily generalizeable to this case.

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Appendix A. some computational details

The numerical code which we have developed is specifically designed for the accurate simulation of a range of capillary flows and incorporates a number of different models which have been proposed for the continuum modelling of dynamic wetting problems; the most complex of these is the interface formation model [6] which requires the solution to a set of partial differential equations on each interface coupled to the bulk flow and the contact angle. Here, we shall describe how the code simulates an unsteady drop spreading, as in Section 6.2; all of the other problems considered in this paper were solved by using a simplified form of this scheme. A more detailed user-friendly step-by-step guide to the entire implementation is given in Sprittles and Shikhmurzaev [19].

We use the finite element method (FEM) which has previously been successfully applied to a range of free surface flows [5,38–40]. More specifically, we use an Arbitrary Lagrangian–Eulerian (ALE) scheme called the Method of Spines [37,41] so that free surface nodes are moved in a Lagrangian manner whilst bulk nodes are evolved in some chosen manner. This has the advantage that, as in the Lagrangian approach, the free surface is captured exactly, whilst keeping the main advantage of Eulerian methods that elements should not become highly distorted. In this method, described in detail in [37], nodes which define the free surface are located at the end of lines along which the bulk nodes are placed. These are the so called spines of the mesh which usually run from a solid surface to the free surface, with nodes spaced between, see Fig. 16. When a free surface node evolves to a new position the whole spine is moved, with the bulk nodes attached. This choice of parameterisation enables simultaneous calculation of the flow field and free surface.

The spines are placed in a manner which is most suitable for the geometry of the problem; we use an approach, initially proposed in [42], which ensures that near the contact line, where we shall require the most resolution, the spines are arcs of circles, whereas as the axis of symmetry is approached the spines become vertical, to match this boundary smoothly. This is achieved by using the

Fig. 16. Left: a mesh generated for a drop spreading problem using the bipolar coordinate system. The diagram shows the mesh after nodes have been attached to the spines and elements tessellated between them. Right: a magnified view of the part indicated on the left; further magnification produces a series of similar diagrams until the minimum mesh size is reached.
bipolar coordinates \((x, \zeta)\) which are related to the Cartesian coordinates \((x, y)\) via the transformation
\[
x = x_c \sinh \chi \cosh \zeta + \cos \chi \cos \zeta, \quad y = x_c \sin \chi \cosh \zeta - \sin \chi \cos \zeta,
\]
where \(\chi \in (0, \infty)\), \(\zeta \in (0, \pi)\) and \((x_c, 0)\) is the position of the contact line. Our mesh is then designed as follows. First we place our spines across the drop by specifying \(\chi\) in such a way that the element size increases as a geometric progression as one moves away from the contact line. The nodes are then placed along each spine using a function for \(\zeta\) which varies from a fixed value at its base to its value at the free surface \(\zeta_f\), which is an unknown of the problem. The elements are then tessellated around the skeleton of the mesh in some appropriate manner and the result is a mesh like the one shown in Fig. 16.

As is relatively standard in the finite element approximation of dynamic wetting flows \([5, 43]\), we use the V6P3 Taylor–Hood triangular elements which approximate the velocity quadratically and the pressure linearly, thus satisfying the Ladyzhenskaya–Babuska–Brezzi constraint \([44]\). Each bulk element contains fifteen unknowns located at six nodes, as shown in Fig. 17. The free surface is approximated quadratically, so that elements which are adjacent to the free surface have one curved side and contain an additional three unknowns specifying the free surface position. Due to the nature of the flow it has been found that, as noted in previous investigations of a similar nature \([5, 45]\), a large number of elements are required in the angular direction near the corner in order to accurately capture the dynamics.

The algebraic finite element equations are derived in a right angled “master” element with local coordinates \((\zeta, \eta)\), see Fig. 17. Inside this element the velocity \(\mathbf{u}\) and pressure \(p\) may be expressed in terms of their nodal values \(\mathbf{u}_n, p_n (j = 1, 6, k = 1, 3)\) by using bi-quadratic \(\phi_i\) and bi-linear \(\psi_k\) interpolating functions, respectively. Then
\[
\mathbf{u} = \sum_{j=1}^{6} \mathbf{u}_j \phi_j(\zeta, \eta), \quad p = \sum_{k=1}^{3} p_k \psi_k(\zeta, \eta).
\]

The same bi-quadratic functions \(\phi_i\) are also used to map the master element with nodal positions \(x_i\) onto the deformed, curved triangular elements in the computational domain via the transformation:
\[
x(\zeta, \eta) = \sum_{j=1}^{6} x_j \phi_j(\zeta, \eta).
\]

The bulk finite element equations are found by substituting equations (30) into the Navier–Stokes equations, see (18), weighting incompressibility by \(\psi_1\) and the momentum equations by \(\psi_3\) then integrating over the entire domain \(\Omega\) and requiring that the resultant expression is zero. We arrive at
\[
\int_{\Omega} \psi_3 \nabla \cdot \mathbf{u} \, d\Omega = 0
\]
and, after using integration by parts and the divergence theorem,
\[
\int_{\Omega} \left( \partial_t \left( \frac{\partial \mathbf{u}}{\partial t} \right) \cdot \nabla \mathbf{u} \right) + Stg + P \cdot \nabla \phi \right) \, d\Omega + \int_{\Gamma_0} \phi_i P \cdot \mathbf{n} \, ds = 0,
\]
where the material derivative takes into account the mesh velocity \(\mathbf{x} = \partial \mathbf{x} / \partial t\), as is required in ALE methods \([46]\); \(\mathbf{n}\) is the inward normal to the boundary \(\partial \Omega\) and \(s\) is the arclength along the boundary.

Boundary conditions of both Dirichlet and stress type are present in our problem formulation. To apply a Dirichlet condition for a given variable we must first identify which equation is used to determine its value, for example the tangential momentum equation determines the tangential velocity \(u_t\) and then replace this equation with the Dirichlet condition at the appropriate node.

Stress conditions are incorporated into the finite element method in a non-intrusive manner by specifying the boundary integral in (33). The only complication here is in implementing the free surface stress conditions \([20]\), which contain second order derivatives of the free surface shape. This is overcome in the standard way by using the Serret–Frenet formula \(\mathbf{v} \cdot \mathbf{n} = dt / ds\), where \(t\) is the tangent vector pointing in the direction of increasing \(s\), and then, following the approach described in Ruschak \([41]\), integrating by parts to give a contribution on the free surface \(\partial \Omega_f\) to the momentum residual (33) of
\[
\int_{\partial \Omega_f} \phi_i P \cdot \mathbf{n} \, ds = \frac{1}{C_a} \left( \int_{\partial \Omega_f} t \frac{d \phi_i}{ds} \, ds - |t|^i \right).
\]

To temporally discretize our equations, we use second-order accurate in time Backward Differentiation Formula (BDF2), which has been applied successfully to similar problems \([47]\). The reader is referred to Gresho and Sani \([48, p. 797]\) for details.

The resulting non-linear equations are solved at each time step using the Newton–Raphson method, with the iterative procedure terminated when the \(L_2\) norm of the residuals falls below \(10^{-8}\). The linearized equations are solved using the MA41 solver provided by the Harwell Subroutine Library.

Finally, we note that in Eq. (10) the pressure is logarithmically singular as the corner is approached and, strictly speaking, one should look to incorporate special ‘singular elements’ there to capture this behaviour \([5]\). The platform we have developed has the option of incorporating these singular elements, and they are investigated in Sprittles and Shikhmurzaev \([20]\). In the results presented here, we have opted against using them in order to simplify our exposition. Their implementation has no effect on the conclusions of this paper, as verified by our test runs.

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