Project 2: Shapes of Liquid Drops

Aim: To write a (approximately) 10 page report that demonstrates:

- engagement with the literature on capillarity,
- computational results for the shapes of drops in different contexts,
- validation of code against your own analytic results as well as experimental/theoretical results from the published literature.

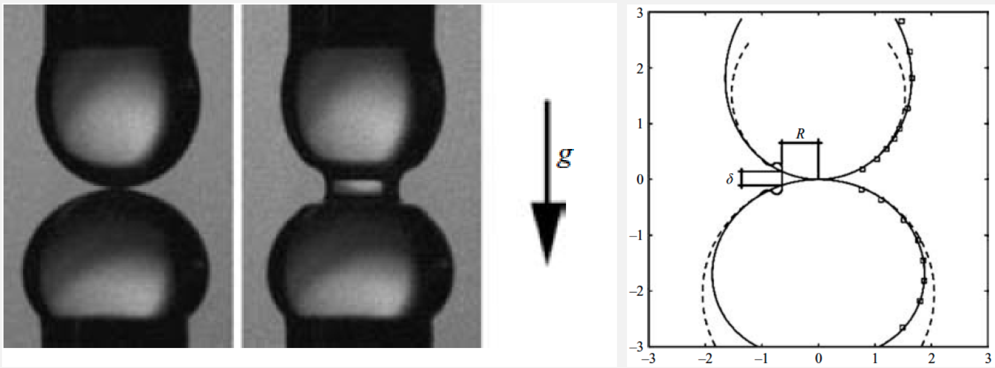

Figure 4.10: Images from Thoroddsen et al's article (see Reading List) showing drops on top of and underneath solid posts experimentally (left) and computed using the Young-Laplace equation (right).

Given Information on Young-Laplace equation in cylindrical polar coordinates
A more realistic drop is obtained if we consider an axisymmetric (nothing depends on θ) drop in a cylindrical polar coordinate system (r, θ, z), so that the equivalent height function is given by $z = h(r)$, where h is the height of the free surface and r is the radial coordinate. In this case we need to know the curvature of our free surface, which is given by (feel free to work this out / check):

$$\nabla \cdot \mathbf{n} = -\frac{r\frac{dh}{dr} + r^2\frac{d^2h}{dr^2}}{r^2\sqrt{1+\left(\frac{dh}{dr}\right)^2}}$$

Project Ideas
The suggestions below are intended to give you ideas of what can be done, but you should feel free to follow your own path if you wish.
A starting point for this project is to compute the static shape of a 2D drop in a gravitational field whose contact line is pinned, as considered within the Week 4 Workshop, where we recall the suggested tasks below.

- Solve the linearised Young-Laplace equation and ensure you get the analytic solution in this case.

- Extend the code to solve the nonlinear problem via iteration and compare for $g = 0$ to (i) the linearised solution for small heights and (ii) the nonlinear solution in all cases.
- Vary P to obtain different drop shapes (for different material parameters, if you like).
- Consider if there is a solution for all values of P. If not, what can go wrong and why?
- Determine the dimensionless parameter appears from the Young-Laplace equation. How do drop shapes vary as you change this parameter?

And also recollect some of the more challenging suggestions for extending the 2D code.

- Can you extend the code to consider prescribing the drop's volume V (or more precisely its area in 2D) and then finding P as part of the solution (hint: you will have to introduce an extra unknown into the problem, namely P, and an additional equation, which is that the drop volume is V and will involve an integral over all nodes)?
- Consider the case of a gas bubble on a solid surface surrounded by an exterior liquid. What changes to the drop shapes?
- Think about implementing the Newton method, which has superior convergence qualities over Picard iteration (error decreases quadratically, rather than linearly). You may have seen this method for the solution of a single equation for a single variable, i.e. $E_1(h_1) = 0$,where we update the values of h_1 using

$$h_1^{k+1} = h_1^k - \frac{E_1(h_1^k)}{\frac{dE_1(h_1^k)}{dh_1}}$$

  and see that the left hand side is the new solution, where the right hand side is evaluated purely at already-existing values. To extend this to a system of equations where we want $E_i(h_1, h_2, ..., h_n) = 0$ at every node, we must use

$$h_i^{k+1} = h_i^k - J_{ij}^{-1} E_j(h_i^k) \qquad J_{ij} = \frac{dE_i(h_i^k)}{dh_j}$$

  and J_{ij}^{-1} is the inverse of J_{ij}. In other words, to find the amount we need to update our solution by $\triangle h_i = h_i^{k+1} - h_i^k$ we must solve the linear equations

$$J_{ij} \triangle h_i = -E_j(h_i^k)$$

Potential extensions are now described - feel free to follow whatever interest you.

Moving contact lines:

- Consider a free (unpinned) contact line, so that R is now an unknown of the problem and a condition is applied on the angle θ at which the free surface meets the solid (see figure 4.8), which can be varied ($h'(x = \pm R) = \mp \tan\theta$). This 'contact angle' can vary from $\theta = 0$, where the drop will completely wet the solid with a thin liquid film, through to $\theta \approx 180°$ where there is almost no contact between the drop and solid (these are 'superhydrophobic surfaces'). Again, you can consider both prescribing P and finding V or vice versa.

Axisymmetric (real) drops:

- Consider 3D axisymmetric drops so that comparisons can be made to experimental data for drops (or bubbles). In this case, the domain will be from $0 \leq r \leq R$, where R is the radial position of the contact line, and at the axis of symmetry ($r = 0$) one has a condition that the free surface is smooth $\frac{dh}{dr} = 0$. Numerically, a crude way to impose this is to enforce that the height of the free surface at the first node h_1 is equal to that at the second node $h_1 = h_2$.
- Attempt to derive an analytic solution in this case for $g = 0$. Noting that the profile is a spherical cap may help.
- Try to compare your drop shapes to those found in the experimental literature (you may find you need to use a fixed contact angle rather than a fixed drop size). You could look into Bonn et al 2009 for ideas/images (see Reading List) or find your own pictures of static drops.

Fat drops:

- Parameterise the free surface so that shapes are not restricted to single valued functions of $h = h(x)$ - i.e. one can consider 'fat drops' like those in Figure 4.10. To do so, one option is to switch to the parameterisation $x = f(y)$, where the f is now the unknown function (perhaps everywhere, or maybe only in regions where this parameterisation suits better). To utilise this approach one need to know the curvature in this representation, which will be easy to obtain in Cartesian coordinates and in cylindrical polar coordinates where $r = f(z)$ will be given by

$$\kappa = \frac{-\frac{d^2 f}{dz^2}}{\left(1 + (\frac{df}{dz})^2\right)^{3/2}} + \frac{1}{f\left(1 + (\frac{df}{dz})^2\right)^{1/2}}.$$

  One needs to be careful near $r = 0$ with this setup.

  An alternative popular approach is to use the arclength coordinate s to find the free surface coordinates as $(r(s), z(s))$. A common way to achieve this was first described by Adams and Bashforth (see Reading List) and can be found more recently in Thoroddsen et al 2005 and Extrand & Moon 2010 as well as no doubt countless other papers. Note that to use this approach one will need to discretise

s rather than x and that the 'shooting method' described in papers is similar to treating s as time and using an explicit stepping method. Note also that here you will have more than one equation at each nodes, but the principles we have developed can still be applied to this new setting (i.e. 3 equations at each node means we will have a $3n \times 3n$ system of equations).

- Extract data from Figure 3 in Thoroddsen et al 2005 (e.g. using DataThief `https://datathief.org/`) and compare to your results. Or try similar approaches with results in Berry et al 2015 (see Reading List), where the Young-Laplace equation is used to determine the surface tension of hanging liquid drops. Similarly you may look into Extrand & Moon 2010 (again in the Reading List).
- Or compare to gas bubble shapes obtained in Simmons et al 2015 in the Reading List below.

For those feeling very ambitious:

- Consider the influence of additional physical effects on drop shapes, for example electric fields (look into the published literature for examples).
- Extend your code to consider quasi-static flows, where the free surface is still computed by the Young-Laplace equation but either (i) for a pinned contact line the volume of the drop changes in time, as in Simmons et al 2015 below, or (ii) there is a relation between the contact angle and the speed of the contact line $U_c = dR/dt$ such as $dR/dt = (\theta^3(t) - \theta_e^3)$. Consider the approach of a drop from some initial shape with angle $\theta_0 = \theta(t = 0)$ towards its equilibrium shape with angle θ_e (at which point $dR/dt = 0$).
- Download and have a play with Surface Evolver `http://facstaff.susqu.edu/brakke/evolver/evolver.html`, which is a code known to accurately compute equilibrium free surface shapes (note: I have never used it, so you are on your own!) . Consider using previous solutions from your own codes as a benchmark and then consider more interesting cases - for example, fully-3D non-axisymmetric cases (e.g. a drop on an inclined plane with a pinned contact line, as you'd see on a car window when it rains).

Reading List
Articles below are just a starting point for your investigations and should not be considered exhaustive

- Pomeau, Y. and Villermaux, E., 2006. Two hundred years of capillarity research. Physics Today, 59(3), p.39.
  History of flows with surface tension considering a range of phenomena. Read for an overview of the topic.

- Bashforth, B., 1883. An attempt to test the theories of capillary action by comparing the theoretical and measured forms of drops of fluid. (with supplement by Adams, J.C.).
  Early attempt to compute the shapes of static drops on or underneath solid surfaces. Quadrature is used to solve the differential equation and this is incredibly laborious in the pre-computer age! Article can be found here: `https://ia800203.us.archive.org/25/items/cu31924012328385/cu31924012328385.pdf`.

- Thoroddsen, S.T., Takehara, K. and Etoh, T.G., 2005. The coalescence speed of a pendent and a sessile drop. Journal of Fluid Mechanics, 527, pp.85-114.
  A paper on the coalescence of liquid drops. Most relevantly, Section 3.1 contains a method for calculating the static shapes of drops using the Young-Laplace equation and Figure 3 shows computed shapes compared to experimental data.

- Bonn, D., Eggers, J., Indekeu, J., Meunier, J. and Rolley, E., 2009. Wetting and spreading. Reviews of modern physics, 81(2), p.739.

- Berry, J.D., Neeson, M.J., Dagastine, R.R., Chan, D.Y. and Tabor, R.F., 2015. Measurement of surface and interfacial tension using pendant drop tensiometry. Journal of colloid and interface science, 454, pp.226-237.
  Method for calculating the surface tension by analysing the shape of a drop and comparing it to the Young-Laplace equation's solutions.

- Simmons, J.A., Sprittles, J.E. and Shikhmurzaev, Y.D., 2015. The formation of a bubble from a submerged orifice. European Journal of Mechanics-B/Fluids, 53, pp.24-36.
  Growth of a gas bubble from a submerged orifice. Here, Section 5.2.1 considers how well the Young-Laplace equation can be used to describe the dynamics (see equation 15 and figure 7), when they are in a quasi-static regime.

- Extrand, C.W. and Moon, S.I., 2010. Contact Angles of Liquid Drops on Super Hydrophobic Surfaces: Understanding the Role of Flattening of Drops by Gravity. Langmuir, 26, pp.17090-17099.
  Article considering how well static drops on superhydrophobic surfaces (those with $\theta \to 180°$) can be described by the Young-Laplace equation. Includes further explanation of method of Adams and Bashforth.