Sample Solutions to HW2

02.Apr.2024

Q1 Meniscus Adjacent to a Wilhelmy Plate

1. Interfacial pressure when $\theta > 90°$

   At the plate the meniscus, we know $p(x = 0) - p_{\text{air}} + 2\mathcal{H}\gamma = 0$. Since $\theta > \pi/2$, the mean principle radius $\mathcal{H} < 0$, therefore we have $p(x = 0) > 1$ atm.

2. Function `f`

   In this question we need to solve a second-order ode equation. First we shall express the ode equation using vector representation, as the skeleton code for function `dHX` as follows (written in the Matlab style):

   The function `f` you need is then to take initial values and put `dHX` into the ode solver:

3. Influence of initial value on the precision of result.

   Ideally, at $X \to \infty$, we have both H and $\frac{\mathrm{d}H}{\mathrm{d}X}$ are 0. Therefore, the values we obtained from the function `f`, represent the error of both H and $\frac{\mathrm{d}H}{\mathrm{d}X}$ at $X = X_{\text{max}}$. Here we plot the absolute errors as functions of the initial guess of H_0, with different choices of X_{max} for the ode that we study, as shown in Figure 1. As can be seen, the absolute error varies dramatically within a certain range (shown in blue shader). The width of such regime also becomes narrower when X_{max} increases. Therefore, the solution of the ODE is greatly influenced by the initial guess of H_0.

4. Dependency of H_0 and θ

   Since both errors of H and $\frac{\mathrm{d}H}{\mathrm{d}X}$ exist, to solve the ode equation, we can use the shooting method to get the correct H_0 value at a certain θ value:

   The solution can be found by non-linear solvers: (e.g. `fsolve` in `Matlab` or `scipy.optimize.fsolve` in `Python`). One thing you need to take care is how to estimate the residue R. To achieve a more stable solution you may want to evaluate both $H(\infty)$ and $\mathrm{d}H/\mathrm{d}X(\infty)$ for R, such as: $R = [H^2(\infty) + (\mathrm{d}H/\mathrm{d}X)^2(\infty)]$. Using the shooting method, we get the dependency of H_0 as function of θ as shown in Figure 2. As can be expected, the height of the meniscus is larger than 0 when $\theta > 0°$, and *vice versa*.

5. Height profiles

   The height profile as function of X can be solved using the ode solver like `ode45` on an array of X values. The result can be seen in Figure 3.

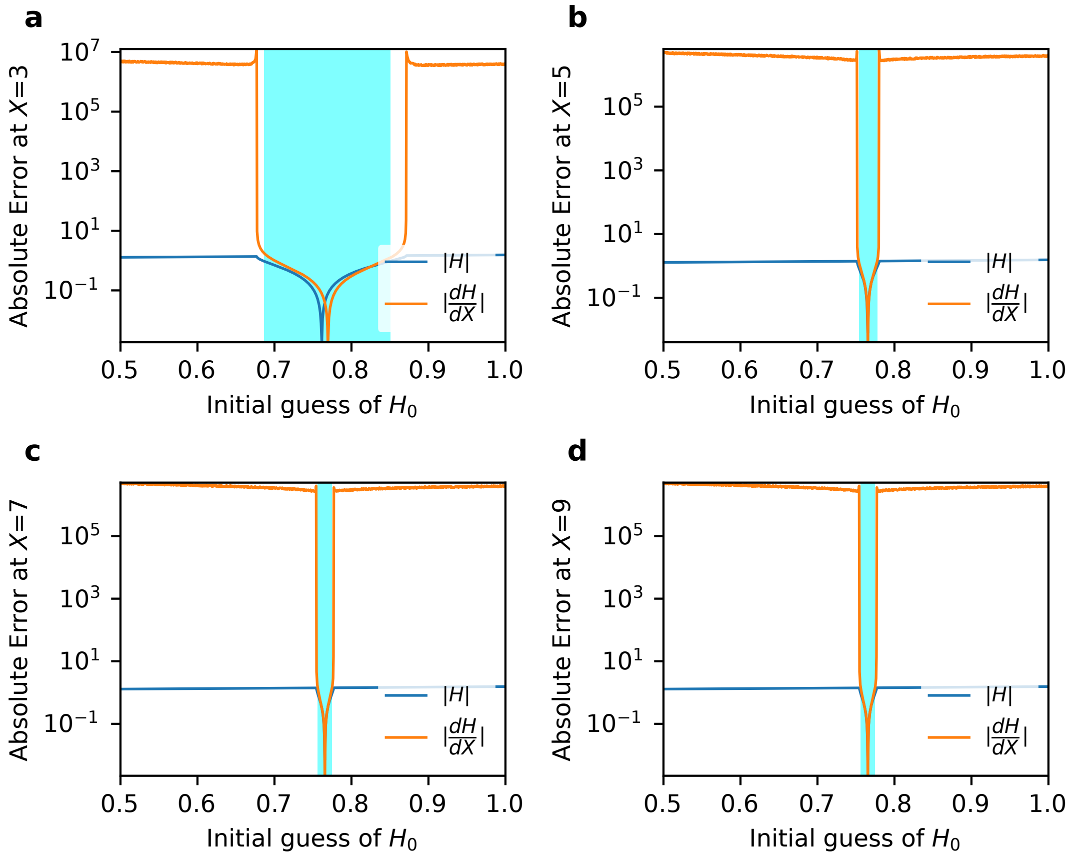

Figure 1: Absolute error of H and $\frac{\mathrm{d}H}{\mathrm{d}X}$ at $X = X_{\max}$, when (a) $X_{\max} = 3$, (b) $X_{\max} = 5$, (c) $X_{\max} = 7$ and (a) $X_{\max} = 9$. The blue shader corresponding to the regime when the error dramatically changes. The answers here are obtained using `scipy.integrate.ode` interface in `Python` with (4)5-order Runge-Kutta algorithm.

Algorithm 1 Pseudo-code for the shooting method

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procedure SHOOTING($\hat{H}_0, \theta_0$)
  $H(0) \leftarrow \hat{H}_0$; $\frac{dH}{dX} \leftarrow -\cot\ \theta_0$ ▷ Initial Guess
  $R \leftarrow$ODE($H(0)$, $\frac{dH}{dX}$)$|_{X\to\infty}$ ▷ Residue
  while $R >$tolerance **do**
    $H(0) \leftarrow H(0) + \delta H$; $\frac{dH}{dX} \leftarrow \frac{dH}{dX} + \delta U$ ▷ Gauss method
    $R \leftarrow$ODE($H(0)$, $\frac{dH}{dX}$)$|_{X\to\infty}$
  end while
  return $H(0)$, R
end procedure

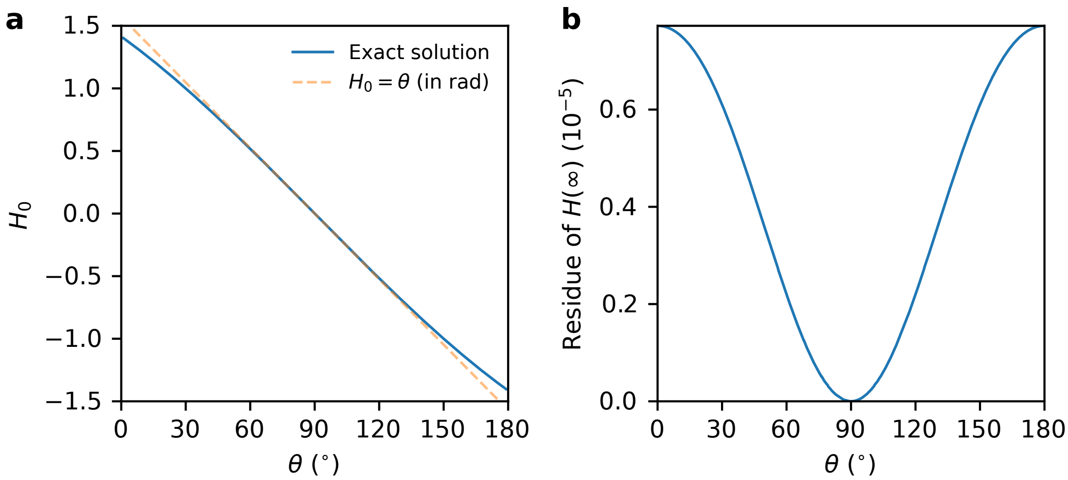

Figure 2: (a) Hight H_0 as a function of θ at the Wilhelmy plate. (b) Residue of the estimation of $H(\infty)$ as a function of θ.

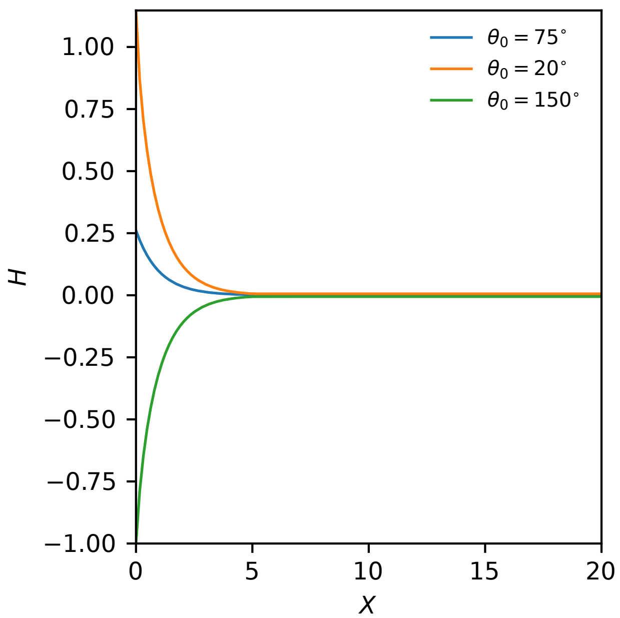

Figure 3: X-dependent height profile of varied contact angles.

As we expected, the meniscus near the plate is higher than 0 for $\theta_0 < 90°$ (hydrophilic). On the other hand the meniscus drops below the liquid surface level for $\theta_0 > 90°$.

Your plots may look different due to difference choice of solver and the conditions you used for the cutoff of "infinite" boundary. Nonetheless in your plot the range of the x axis should not exceed your cutoff value. Otherwise you will see a rise of the meniscus due to error accumulation in the ode solving process.

To get an accurate solution, some caution should be taken for the initial guess of H_0. One trick is as follows;

(a) Get the solution of H_0 when $\theta = 90°$ (is 0!)

(b) Use the solution of H_0 you get from step 1 as the initial guess for angles $\theta \pm \delta\theta$. $\delta\theta$ is a small angle (for instance 0.5 °)

(c) Repeat steps 1 and 2 until you get the solution for the angle you want to study.

By making $\delta\theta$ smaller, you have higher chance to obtain a stable solution.

6. Comparing the analytical and numerical solutions

   The numerical and analytical solution for cases $\theta_0 = 20°$ and $\theta_0 = 75°$ can be seen in Figure 4. With the offset of X_0 we see that our numerical solution is in perfect agreement with the analytical one.

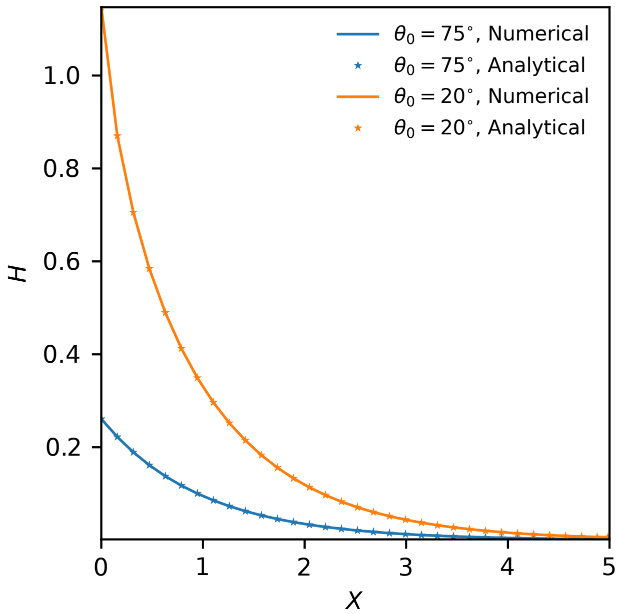

Figure 4: Comparison between the numerical and analytical solutions when $\theta_0 = 20°$ and $\theta_0 = 75°$

Q2 Growth of Ice Crystal in Salt Water

1. Interface salt concentration

   Since salt does not dissolve in solid, salt will be ejected upon ice growth, so $C_{IL} > C_\infty$ would occur.

2. Interface heat balance

   The heat balance at interface follows

$$\rho\lambda\frac{da}{dt} = -k_L\frac{dT_L}{dx}$$

   Using the temperature profiles, it follows

$$\rho\lambda\frac{da}{dt} = -k_L\frac{T_\infty - T_F(t)}{\delta}$$

   Note that now it becomes an ODE with two unknowns $a(t)$ and $T_F(t)$.

3. Interface concentration balance

   The concentration balance at interface follows

$$C_{IL}(t)\frac{da}{dt} = -D_L\frac{dC_L}{dx}$$

   Using the temperature profiles, it follows

$$C_{IL}(t)\frac{da}{dt} = -D_L\frac{[C_\infty - CIL(t)]}{\delta}$$

   Note that now it becomes an ODE with two unknowns $a(t)$ and $C_{IL}(t)$.

4. Heat and mass transfer equations

   We have three unknown functions as functions of t, $a(t)$, $T_F(t)$, and $C_{IL}(t)$, and three equations as follows.

$$\rho\lambda\frac{da}{dt} = -k_L\frac{[T_\infty - T_F(t)]}{\delta} \tag{1}$$

$$C_{IL}(t)\frac{da}{dt} = -D_L\frac{[C_\infty - C_{IL}(t)]}{\delta} \tag{2}$$

$$T_F(t) = T_0 - \beta C_{IL}(t) \tag{3}$$

   Accordingly we can solve the ODEIVPs using matlab with the following initial values: $a(t) = 0$, $T_F(0) = T_W$ and $C_{IL}(0) = C_\infty$