Numerical Methods

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1 Mappings and notations

We are considering the 2-D case with the mapping

$$x = X \tag{1}$$
$$z = F(X, Z, \tau) \tag{2}$$
$$t = \tau \tag{3}$$

where

$$F(X, Z, \tau) \triangleq \begin{cases} Z + h(X,\tau)\, exp(-\alpha Z), & Z \geq 0 \\ Z + h(X,\tau)\, exp(\alpha Z), & Z \leq 0 \end{cases} \tag{4}$$

If we define

$$G_0 = \frac{F_\tau}{F_Z}\,, \qquad G_1 = \frac{F_X}{F_Z}\,, \qquad G_3 = \frac{1}{F_Z} \tag{5}$$

then

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial \tau} - G_0 \frac{\partial}{\partial Z} \tag{6}$$
$$\frac{\partial}{\partial x} = \frac{\partial}{\partial X} - G_1 \frac{\partial}{\partial Z} \tag{7}$$
$$\frac{\partial}{\partial z} = G_3 \frac{\partial}{\partial Z} \tag{8}$$
$$\frac{\partial^2}{\partial x^2} = \frac{\partial^2}{\partial X^2} + (G_1)^2 \frac{\partial^2}{\partial Z^2} - 2G_1 \frac{\partial^2}{\partial X \partial Z} + (G_1 (G_1)_Z - (G_1)_X) \frac{\partial}{\partial Z} \tag{9}$$
$$\frac{\partial^2}{\partial z^2} = (G_3)^2 \frac{\partial^2}{\partial Z^2} + G_3 (G_3)_Z \frac{\partial}{\partial Z} \tag{10}$$

Let's further define

$$g_2 = (G_1)^2 + (G_3)^2\,, \quad g_3 = -2G_1\,, \quad g_4 = G_1 \frac{\partial G_1}{\partial Z} + G_3 \frac{\partial G_3}{\partial Z} - \frac{\partial G_1}{\partial X} \tag{11}$$

Then we can write the Laplacian in new variables as

$$\begin{aligned} \mathcal{L} &\triangleq \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} \\ &= \frac{\partial^2}{\partial X^2} + g_2 \frac{\partial^2}{\partial Z^2} + g_3 \frac{\partial^2}{\partial X \partial Z} + g_4 \frac{\partial}{\partial Z} \end{aligned} \tag{12}$$

Remarks:

1. In the upper domain ($Z \geq 0$) and the lower domain ($Z \leq 0$), each of G_i ($i = 0, 1, 3$), g_i ($i = 2, 3, 4$) has different expressions, corresponding to (4).

2. In particular, if we set $\alpha = 0$ in (4), we get, in both domains,

$$G_0 = h_\tau \ , \quad G_1 = h_X \ , \quad G_3 = 1 \ ; \tag{13}$$

$$g_2 = 1 + (h_X)^2 \ , \quad g_3 = -2h_X \ , \quad g_4 = -h_{XX} \tag{14}$$

This is called the simple mapping.

2 Numerical methods

With the mappings, the governing equations as well as the interfacial conditions are given in Euqations (3.1)-(3.4) in Dr. Baker's notes: Mapped Equations. Here we rewrite those equations with a few changes:

i) we introduce the generalized pressure $P = p + \rho g z$ so that the gravity g doesn't appear in the governing equation (3.1b). Instead, it appears in the stress condition (3.4b).

ii) By using the incompressiblity condition (3.1c), we eliminate $w_Z^{(1)}$ and $w_Z^{(2)}$ in the stress conditions (3.4a) and (3.4b).

The momemtum equations are now:

$$u_\tau - G_0 u_Z + u(u_X - G_1 u_Z) + w G_3 u_Z = -\frac{1}{\rho} P_X + \frac{1}{\rho} G_1 P_Z + \nu \mathcal{L}\{u\} \tag{15}$$

$$w_\tau - G_0 w_Z + u(w_X - G_1 w_Z) + w G_3 w_Z = -\frac{1}{\rho} G_3 P_Z + \nu \mathcal{L}\{w\} \tag{16}$$

and the incompressibility condition is

$$u_X - G_1 u_Z + G_3 w_Z = 0 \tag{17}$$

At the interface, we have continuity of the velocity

$$u^{(1)} = u^{(2)} = u^{(I)} \ , \quad w^{(1)} = w^{(2)} = w^{(I)} \tag{18}$$

and the kinamatic condition

$$h_\tau + u^{(I)} h_X = w^{(I)} \tag{19}$$

The stress conditions (or dynamic interfacial condtions) are now:

$$\begin{aligned} \mu^{(1)}(G_3^{(1)} u_Z^{(1)} + w_X^{(1)}) &- \mu^{(2)}(G_3^{(2)} u_Z^{(2)} + w_X^{(2)}) + (\frac{4h_X}{h_X^2 - 1} + \frac{G_1^{(1)}}{G_3^{(1)}}) \mu^{(1)}(u_X^{(1)} - G_1^{(1)} u_Z^{(1)}) \\ &- (\frac{4h_X}{h_X^2 - 1} + \frac{G_1^{(2)}}{G_3^{(2)}}) \mu^{(2)}(u_X^{(2)} - G_1^{(2)} u_Z^{(2)}) = 0 \end{aligned} \tag{20}$$

$$\begin{aligned} (P^{(1)} - P^{(2)}) &+ (2 - \frac{4h_X^2}{h_X^2 - 1})[\mu^{(1)}(u_X^{(1)} - G_1^{(1)} u_Z^{(1)}) - \mu^{(2)}(u_X^{(2)} - G_1^{(2)} u_Z^{(2)})] \\ &= gh(\rho^{(1)} - \rho^{(2)}) + 2T\kappa \end{aligned} \tag{21}$$

Note that, we have used (20) to obtain (21).

The numerical methods to be applied are as follows.

1. For the time discretization, we use the Crank-Nicolson method to treat the linearized terms and the Adam-Bashforth method to all the other (nonlinear) terms.

2. We introduce a new variable $q = u_Z$. Then we write the governing equations into a 4 by 4 system of 1st-order ODEs

$$\frac{d}{dZ}Y \;=\; BY + R \tag{22}$$

wehre $Y \triangleq \begin{pmatrix} u^{n+1} \\ q^{n+1} \\ w^{n+1} \\ p^{n+1} \end{pmatrix}$ are the solutions at the new time level n+1, where B is a 4 by 4 constant matrix and where $R \triangleq \begin{pmatrix} R_1 \\ R_2 \\ R_3 \\ R_4 \end{pmatrix}$ is a vector. Both B and R are determined by the time discretization methods. Numerically, (22) must be solved at each grid point in the vertical direction. Importantly, boundary conditions are needed to complete the system.

3. With the assumption that solutions are periodic in the X-direction, we can take advantage of the discrete Fourier transform. Then it's sufficient to solve (22) for each Fourier mode k, i.e.,

$$\frac{d}{dZ}Y_k \;=\; B_k Y_k + R_k\,, \quad k = 0, 1, \cdots, K-1 \tag{23}$$

with corresponding boundary conditions. (From now on we use the subscript k to denote the k-th Fourier coefficient.)

4. An ODE solver is then applied to effectively solve the system (23) to give the solutions Y_k.

Details for the above ideas follow.

2.1 Calculation of B and R

Firstly, we have $u_Z = q$, which gives the equation at the time step n+1,

$$u_Z^{n+1} - q^{n+1} = 0 \tag{24}$$

Hence $R_1 = 0$.

Secondly, from the momemtum equation (15) we have (In all the following equations, we replace u_Z by q.)

$$\begin{aligned} u_\tau + \frac{1}{\rho}P_X - \nu(u_{XX} + q_Z) \;&=\; G_0 q + \frac{1}{\rho}G_1 P_Z - [u(u_X - G_1 q) + wG_3 q] + \nu[(g_2-1)q_Z + g_3 q_X + g_4 q] \\ &\triangleq\; R_u \end{aligned} \tag{25}$$

Applying the Crank-Nicolson for the left-hand side and the Adam-Bashforth for the right-hand side, we get

$$\frac{u^{n+1} - u^n}{\Delta\tau} + \frac{1}{2\rho}(P_X^{n+1} + P_X^n) - \frac{\nu}{2}(u_{XX}^{n+1} + q_Z^{n+1} + u_{XX}^n + q_Z^n) = \frac{3}{2}R_u^n - \frac{1}{2}R_u^{n-1} \tag{26}$$

After collecting terms and multiplying $-\frac{2}{\nu}$ at both sides, we obtain

$$q_Z^{n+1} - \frac{2}{\nu}(\frac{u^{n+1}}{\Delta\tau} - \frac{\nu}{2}u_{XX}^{n+1}) - \frac{1}{\rho\nu}P_X^{n+1} = -\frac{2}{\nu}[\frac{3}{2}R_u^n - \frac{1}{2}R_u^{n-1} + (\frac{u^n}{\Delta\tau} - \frac{1}{2\rho}P_X^n + \frac{\nu}{2}(u_{XX}^n + q_Z^n))] \quad (27)$$

The right-hand side of (27) gives R_2.

Thirdly, the incompressibility condition (17) gives

$$u_X + w_Z = G_1 q + (1 - G_3)w_Z \quad (28)$$

Using the 2nd-order extrapolation for the right-hand side at the time step n+1, we obtain

$$w_Z^{n+1} + u_X^{n+1} = 2(G_1^n q^n + (1 - G_3^n)w_Z^n) - (G_1^{n-1}q^{n-1} + (1 - G_3^{n-1})w_Z^{n-1}) \quad (29)$$

The right-hand side of (29) gives R_3.

Finally, from the momentum equation (16) we have

$$\begin{aligned} w_\tau + \frac{1}{\rho}P_Z - \nu(w_{XX} + w_{ZZ}) &= G_0 w_Z + \frac{1}{\rho}(1 - G_3)P_Z - [u(w_X - G_1 w_Z) + wG_3 w_Z] \\ &\quad +\nu[g_2 w_{ZZ} + g_3 w_{XZ} + g_4 w_Z - w_{ZZ}] \end{aligned} \quad (30)$$

we don't want the w_{ZZ} term on the left-hand side since it's a 2nd-order derivative with respect to Z. We note that, in the case of flat interface the incompressibility condition reads

$$u_X + w_Z = 0 \quad (31)$$

which implies

$$w_{ZZ} + u_{XZ} = 0\,, \quad \text{or} \quad w_{ZZ} + q_X = 0 \quad (32)$$

Hence, we can replace w_{ZZ} by $-q_X$ on the left-hand side of (30) and modify the right-hand side accordingly,

$$\begin{aligned} w_\tau + \frac{1}{\rho}P_Z - \nu(w_{XX} - q_X) &= G_0 w_Z + \frac{1}{\rho}(1 - G_3)P_Z - [u(w_X - G_1 w_Z) + wG_3 w_Z] \\ &\quad +\nu[g_2 w_{ZZ} + g_3 w_{XZ} + g_4 w_Z + q_X] \\ &\triangleq R_w \end{aligned} \quad (33)$$

Applying the Crank-Nicolson for the left-hand side and the Adam-Bashforth for the right-hand side, we get

$$\frac{w^{n+1} - w^n}{\Delta\tau} + \frac{1}{2\rho}(P_Z^{n+1} + P_Z^n) - \frac{\nu}{2}(w_{XX}^{n+1} - q_X^{n+1} + w_{XX}^n - q_X^n) = \frac{3}{2}R_w^n - \frac{1}{2}R_w^{n-1} \quad (34)$$

After collecting terms and multiplying 2ρ at both sides, we obtain

$$P_Z^{n+1} + 2\rho(\frac{w^{n+1}}{\Delta\tau} - \frac{\nu}{2}w_{XX}^{n+1}) + \rho\nu q_X^{n+1} = 2\rho[\frac{3}{2}R_w^n - \frac{1}{2}R_w^{n-1} + (\frac{w^n}{\Delta\tau} - \frac{1}{2\rho}P_Z^n + \frac{\nu}{2}(w_{XX}^n - q_X^n))] \quad (35)$$

The right-hand side of (35) gives R_4.

Then it's ready to apply the Fourier transform along the X-direction to the above equations (24)(27)(29)(35). For the left-hand sides of these equations, we simply replace $\frac{\partial}{\partial x}$ by ik, $\frac{\partial^2}{\partial x^2}$ by

$-k^2$. For the right-hand sides, we carry out the pseudo-spectral approach (i.e., go back to the physical space to do the products) to obtain $(R_1)_k, (R_2)_k, (R_3)_k, (R_4)_k$, respectively.

Then it's readily seen that

$$B_k = \begin{bmatrix} 0 & 1 & 0 & 0 \\ \frac{1}{\nu\Delta\tau}(2+\nu k^2\Delta\tau) & 0 & 0 & \frac{1}{\rho\nu}ik \\ -ik & 0 & 0 & 0 \\ 0 & -\rho\nu ik & -\frac{\rho}{\Delta\tau}(2+\nu k^2\Delta\tau) & 0 \end{bmatrix} \tag{36}$$

we can also work out the 4 eigenvalues of B_k, which are given by

$$\lambda_1 = k\ , \quad \lambda_2 = -k\ , \quad \lambda_3 = \psi_k\ , \quad \lambda_4 = -\psi_k \tag{37}$$

where $\psi_k \triangleq \sqrt{k^2 + \frac{2}{\nu\Delta\tau}}$.

2.2 The interfacial conditions

The system (22) or (23) holds in both the air and the water. Their solutions are conneceted through the jump conditions across the interface. In the context of (22), the interfacial conditions can be written as

$$T^{(1)} \begin{pmatrix} u^{(1)} \\ q^{(1)} \\ w^{(1)} \\ P^{(1)} \end{pmatrix} - T^{(2)} \begin{pmatrix} u^{(2)} \\ q^{(2)} \\ w^{(2)} \\ P^{(2)} \end{pmatrix} = S \quad \text{or} \quad T^{(1)}Y^{(1)} - T^{(2)}Y^{(2)} = S \tag{38}$$

where the superscripts (1),(2) denote the upper domain (air) and the lower domain (water), respectively. T is a 4 by 4 constant matrix and $S \triangleq \begin{pmatrix} S_1 \\ S_2 \\ S_3 \\ S_4 \end{pmatrix}$ is a vector. After the Fourier transform, we'll get the jump conditions for each Fourier mode k ($k = 0, 1, \cdots, K-1$)

$$T_k^{(1)}Y_k^{(1)} - T_k^{(2)}Y_k^{(2)} = S_k \tag{39}$$

which corresponds to (23). Now we determine T, S.

Firstly, we have the continuity of the velocity u, which reads

$$(u^{n+1})^{(1)} - (u^{n+1})^{(2)} = 0 \tag{40}$$

Hence $S_1 = 0$.

Secondly, we consider the 1st stress condition (20), which gives

$$\begin{aligned} \mu^{(1)}(q^{(1)} + w_X^{(1)}) - \mu^{(2)}(q^{(2)} + w_X^{(2)}) &= \mu^{(1)}(1 - G_3^{(1)})q^{(1)} - \mu^{(2)}(1 - G_3^{(2)})q^{(2)} \\ &\quad -(\frac{4h_X}{h_X^2 - 1} + \frac{G_1^{(1)}}{G_3^{(1)}})\mu^{(1)}(u_X^{(1)} - G_1^{(1)}q^{(1)}) \\ &\quad +(\frac{4h_X}{h_X^2 - 1} + \frac{G_1^{(2)}}{G_3^{(2)}})\mu^{(2)}(u_X^{(2)} - G_1^{(2)}q^{(2)}) \\ &\triangleq r_2 \end{aligned} \tag{41}$$

The left-hand side of (41) is evaluated at the time level n+1 and the right-hand side is extrapolated by $r_2^{n+1} = 2r_2^n - r_2^{n-1}$. Hence

$$S_2 = 2r_2^n - r_2^{n-1} \tag{42}$$

Thirdly, we have the continuity of the velocity w, which reads

$$(w^{n+1})^{(1)} - (w^{n+1})^{(2)} = 0 \tag{43}$$

Hence $S_3 = 0$.

Finally, we consider the 2nd stress condition (21), which gives

$$\begin{aligned}(P^{(1)} - P^{(2)}) + 2(\mu^{(1)}u_X^{(1)} - \mu^{(2)}u_X^{(2)}) &= gh(\rho^{(1)} - \rho^{(2)}) + 2T\kappa \\ &\quad +2(\mu^{(1)}G_1^{(1)}q^{(1)} - \mu^{(2)}G_1^{(2)}q^{(2)}) \\ &\quad +\frac{4h_X^2}{h_X^2 - 1}[\mu^{(1)}(u_X^{(1)} - G_1^{(1)}q^{(1)}) - \mu^{(2)}(u_X^{(2)} - G_1^{(2)}q^{(2)})] \\ &\triangleq r_4\end{aligned} \tag{44}$$

The left-hand side of (44) is evaluated at the time level n+1 and the right-hand side is extrapolated by $r_4^{n+1} = 2r_4^n - r_4^{n-1}$. Hence

$$S_4 = 2r_4^n - r_4^{n-1} \tag{45}$$

Then we can readily apply the Fourier transform to obtain $(S_1)_k$, $(S_2)_k$, $(S_3)_k$, $(S_4)_k$, respectively, and get

$$T_k = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \mu & ik\mu & 0 \\ 0 & 0 & 1 & 0 \\ 2ik\mu & 0 & 0 & 1 \end{pmatrix} \tag{46}$$

2.3 The transformed system

To find an effective ODE solver for (23), we transform it into a diagonal (when $k \neq 0$) or bi-diagonal (when $k = 0$) system

$$\frac{d}{dZ}y_k = \Gamma_k y_k + Q_k^{-1}R_k \tag{47}$$

where

$$y_k \triangleq Q_k^{-1}Y_k\ , \quad \Gamma_k \triangleq Q_k^{-1}B_kQ_k = \begin{cases} \begin{pmatrix} k & & & \\ & -k & & \\ & & \psi_k & \\ & & & -\psi_k \end{pmatrix} & , k \neq 0 \\ \begin{pmatrix} 0 & 1 & & \\ & 0 & & \\ & & \psi_0 & \\ & & & -\psi_0 \end{pmatrix} & , k = 0 \end{cases}$$

(see (37) for ψ_k) and where Q_k can be chosen to be

$$\begin{bmatrix} k & 1 & \psi_k & 1 \\ k^2 & -k & \psi_k^2 & -\psi_k \\ -ik & i & -ik & \frac{ik}{\psi_k} \\ \frac{2\rho i}{\Delta\tau} & \frac{2\rho i}{k\Delta\tau} & 0 & 0 \end{bmatrix} \quad \text{for } k \neq 0$$

and

$$\begin{bmatrix} 0 & 0 & \psi_0 & 1 \\ 0 & 0 & \psi_0^2 & -\psi_0 \\ 0 & -\frac{\Delta\tau}{2\rho} & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \quad \text{for } \ k=0$$

Furthermore, Q_k^{-1} is obtained by solving a linear system via Gaussian Elimination.

At the interface, the jump condition (39) is transformed into

$$T_k^{(1)}Q_k^{(1)}y_k^{(1)} - T_k^{(2)}Q_k^{(2)}y_k^{(2)} = S_k \tag{48}$$

2.4 The ODE solver

Under the transform (47), the system is reduced to 4 scalar equations, for which a couple of scalar ODE solver can be applied. It's not clear yet what's the best choice. One idea we are trying is as follows.

Consider a scalar ODE

$$\frac{d}{dZ}f = \lambda f + b(Z) \tag{49}$$

where f represents one component of y_k and $b(Z)$ one component of $Q_k^{-1}R_k$. Multiply $e^{-\lambda Z}$ at both sides of (49) to obtain

$$\frac{d}{dZ}(e^{-\lambda Z}f) = e^{-\lambda Z}b(Z) \tag{50}$$

Apply the Trapezoid rule to obtain

$$\frac{e^{-\lambda Z_{j+1}}f_{j+1} - e^{-\lambda Z_j}f_j}{\Delta Z} = \frac{1}{2}(e^{-\lambda Z_{j+1}}b_{j+1} + e^{-\lambda Z_j}b_j) \tag{51}$$

If $\lambda < 0$, we use

$$f_{j+1} = e^{\lambda\Delta Z}f_j + \frac{\Delta Z}{2}(b_{j+1} + e^{\lambda\Delta Z}b_j)\ , \quad j = -J, -J+1, \cdots, -1 \tag{52}$$

That means we start from the bottom and go up by the formula (52) until we reach the interface. The bottom boundary conditions should be prescribed in this case.

If $\lambda > 0$, we use

$$f_j = e^{-\lambda\Delta Z}f_{j+1} - \frac{\Delta Z}{2}(e^{-\lambda\Delta Z}b_{j+1} + b_j)\ , \quad j = J, J-1, \cdots, 1 \tag{53}$$

That means we start from the top and go down by the formula (53) until we reach the interface. The top boundary conditions should be prescribed in this case.

For the case $k \neq 0$ in our system, we have 2 positive eigenvalues $\lambda = k,\ \psi_k$ and 2 negative eigenvalues $\lambda = -k,\ -\psi_k$. Hence, the solver for our ODE system has 4 threads, 2 threads following the pattern of (52) and the other 2 the pattern of (53). At the interface, the jump condition (48) is applied and we solve a 4 by 4 linear system. Then we continue the computation on each thread until we reach the top ($\lambda < 0$) or the bottom ($\lambda > 0$).

The idea is essentially the same with the case $k = 0$. The only difference is that, we now have 2 zero eigenvalues and we have to start the 2 corresponding threads from the same place, either the top or the bottom.

2.5 The logical process in codes

We code up the above ideas as follows.

1. Initialize u, q, w, P and h by the linearized solutions given in Notes: Laminar Flow. To prepare for that, the Newton's method is applied to numerically find the roots of σ.

2. At each time step n+1, do the following:

(2.1) Calculate the righ-hand sides for the governing system and the interfacial conditions, i.e., R and S (actually R_k and S_k), respectively, by using the solutions at the time steps n and n-1.

(2.2) Update the interface shape by the kinematic condition (19). Numerically, we use the Adam-Bashforth method to discretize (19),

$$\frac{h^{n+1} - h^n}{\Delta\tau} = \frac{3}{2}(w^{(I)} - u^{(I)}h_X)^n - \frac{1}{2}(w^{(I)} - u^{(I)}h_X)^{n-1} \tag{54}$$

which is carried out in the Fourier space for each mode k.

(2.3) For each mode k, call the ODE solver to solve the transformed system to obtain y_k^{n+1} .

(2.4) Recover the original variables by $Y_k^{n+1} = Q_k y_k^{n+1}$.

(2.5) go to next time step.