Numerical solution of a nonlinear thin-film equation: gravity-driven spreading of a thin film with surface tension over a horizontal substrate

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1 References

J Lopez, *Dynamics of wetting processes*, Ph.D. Thesis (Carnegie Mellon University), (1975)
D U von Rosenberg, *Methods for the Numerical Solution of Partial Differential Equations* (1969)

2 Basic equations (dimensionAL form)

$$\frac{\partial h}{\partial t} = \frac{1}{\sigma}\frac{\partial}{\partial \sigma}\left(\sigma \frac{h^3}{3\mu}\frac{\partial P}{\partial \sigma}\right) \tag{2.1}$$

$$P = \rho g h - \frac{\gamma}{\sigma}\frac{\partial}{\partial \sigma}\left(\sigma \frac{\partial h}{\partial \sigma}\right) + \frac{A}{6\pi h^3} \tag{2.2}$$

$$h(\sigma, 0) = h(\sigma) \tag{2.3}$$

$$\frac{\partial h}{\partial \sigma}(0, t) = 0 \tag{2.4}$$

$$\frac{\partial P}{\partial \sigma}(0, t) = 0 \tag{2.5}$$

$$h[r(t), t] = h^* \tag{2.6}$$

$$\frac{\partial h}{\partial \sigma}[r(t), t] = -\alpha \tag{2.7}$$

$$2\pi \int_0^{r(t)} h(\sigma, t)\, \sigma \, \mathrm{d}\sigma = \mathit{\Omega} \tag{2.8}$$

where t is time, σ is the radial position h is the film thickness, P is the pressure, γ is the surface tension, ρ the density, g the acceleration due to gravity, μ the viscosity, A the Hamaker constant, α the contact slope, h^* the contact height, Ω the drop volume, and r the drop radius.

2.1 Reformulation of the free-boundary problem

The boundary $\sigma = r(t)$ is free. Need to redefine the problem on a fixed domain.

Define the modified coordinates:

$$\xi(\sigma, t) = \frac{\sigma}{r(t)}, \qquad \tau(t) = \frac{t}{[r(t)]^2}$$

By the chain rule,

$$\frac{\partial}{\partial \sigma} = \frac{1}{r}\frac{\partial}{\partial \xi}, \qquad \frac{\partial}{\partial t} = \frac{1}{r^2}\left(1 - \frac{2t}{r}\frac{\mathrm{d}r}{\mathrm{d}t}\right)\frac{\partial}{\partial \tau} = \frac{1}{r^2}\left(1 - \frac{2\tau}{r}\frac{\partial r}{\partial \tau} + O[(\partial r/\partial \tau)^2]\right)\frac{\partial}{\partial \tau},$$

$$\int_0^{r(t)} (\,\cdot\,)\,\sigma\,\mathrm{d}\sigma = r^2 \int_0^1 (\,\cdot\,)\,\xi\,\mathrm{d}\xi$$

Thus, we obtain the modified problem:

$$d(\tau)\frac{\partial h}{\partial \tau} = \frac{1}{\xi}\frac{\partial}{\partial \xi}\left(\xi k(h)\frac{\partial p}{\partial \xi}\right) \tag{2.9}$$

$$p = h - \frac{\lambda^2}{r^2}\frac{1}{\xi}\frac{\partial}{\partial \xi}\left(\xi\frac{\partial h}{\partial \xi}\right) + \frac{\kappa}{h^3} \tag{2.10}$$

$$h(\xi, 0) = h(\xi) \tag{2.11}$$

$$\frac{\partial h}{\partial \xi}(0, \tau) = 0 \tag{2.12}$$

$$\frac{\partial p}{\partial \xi}(0, \tau) = 0 \tag{2.13}$$

$$h(1, \tau) = h^* \tag{2.14}$$

$$\frac{\partial h}{\partial \xi}(1, \tau) = -\alpha r \tag{2.15}$$

$$2\pi r^2 \int_0^1 h(\xi, \tau)\,\xi\,\mathrm{d}\xi = \mathit{\Omega} \tag{2.16}$$

where

$$p = \frac{P}{\rho g}, \quad \lambda^2 = \frac{\gamma}{\rho g}, \quad \kappa = \frac{A}{6\pi\rho g}, \quad d(\tau) = 1 - \frac{\mathrm{d}r^2}{\mathrm{d}t}\tau, \quad k(h) = \frac{\rho g h^3}{3\mu}$$

We needed to transform the time derivative so that the spreading velocity appears explicitly in the equation. At each timestep, we update the spreading distance using the computed velocity.

Note that the integral constraint is used to solve for the free boundary $r(\tau)$.

3 Finite difference analogy

Discretize $\{\xi_j\}$, $\{\tau_n\}$, $j = 0, 1, \ldots, J$, $n = 0, 1, \ldots, N$ on a uniform grid, where $\xi_j = j\Delta\xi$ and $\tau_n = n\Delta\tau$. Shift h and p by 1/2 step in space, so that $h_{j,n} = h(\xi_{j+\frac{1}{2}}, t_n)$ and $p_{j,n} = p(\xi_{j+\frac{1}{2}}, t_n)$.

This is useful for two reasons. Firstly, the BCs can be easily applied. Second, we avoid the singularity at $\xi = 0$.

For now, ignore the van der Waals term in the equation for the pressure (i.e. set $\kappa = 0$). Might find that we are unable to satisfy the right BC $h = 0$ at $\xi = 1$, but let's find out later...

3.1 Boundary conditions

$$\frac{h_{0,n} - h_{-1,n}}{\Delta\xi} = 0 \tag{3.1}$$

$$\frac{p_{0,n} - p_{-1,n}}{\Delta\xi} = 0 \tag{3.2}$$

$$\frac{h_{J-1,n} + h_{J,n}}{2} = h^* \tag{3.3}$$

$$\frac{h_{J,n} - h_{J-1,n}}{\Delta\xi} = -\alpha r_n \tag{3.4}$$

$$\pi r_n^2 \Delta\xi^2 \left[J h^* + \sum_{j=1}^{J-1} j(h_{j-1,n} + h_{j,n}) \right] = \Omega \tag{3.5}$$

from which we obtain

$$h_{-1,n} = h_{0,n} \tag{3.6}$$

$$p_{-1,n} = p_{0,n} \tag{3.7}$$

$$h_{J-1,n} = h^* + \frac{\alpha r_n \Delta\xi}{2} \tag{3.8}$$

$$h_{J,n} = h^* - \frac{\alpha r_n \Delta\xi}{2} \tag{3.9}$$

$$r_n = \left[\frac{\Omega}{\pi \Delta\xi^2 \left[J h^* + \sum_{j=1}^{J-1} j(h_{j-1,n} + h_{j,n}) \right]} \right]^{\frac{1}{2}} \tag{3.10}$$

Thus we eliminate $h_{-1,n}$, $h_{J-1,n}$, and $h_{J,n}$ as unknowns.

3.2 Centered difference analogs for $2 \leq j \leq J-4$

Centered difference equations at $\xi_{j+\frac{1}{2}}$, $\tau_{n+\frac{1}{2}}$ (note that $h_{j,n+\frac{1}{2}}$, $p_{j,n+\frac{1}{2}}$ corresponds to the physical point $\xi_{j+\frac{1}{2}}, \tau_{n+\frac{1}{2}}$):

$$d_{n+\frac{1}{2}} \frac{h_{j,n+1} - h_{j,n}}{\Delta\tau} = \frac{1}{(j+\frac{1}{2})\Delta\xi^2} \left[(j+1)\Delta\xi k_{j+\frac{1}{2},n+\frac{1}{2}} \left(\frac{p_{j+1,n+\frac{1}{2}} - p_{j,n+\frac{1}{2}}}{\Delta\xi} \right) \right. \\ \left. - j\Delta\xi k_{j-\frac{1}{2},n+\frac{1}{2}} \left(\frac{p_{j,n+\frac{1}{2}} - p_{j-1,n+\frac{1}{2}}}{\Delta\xi} \right) \right] \tag{3.11}$$

$$p_{j,n+\frac{1}{2}} = h_{j,n+\frac{1}{2}} - \frac{\lambda^2}{(j+\frac{1}{2})r^2_{n+\frac{1}{2}}\Delta\xi^2}\left[(j+1)\Delta\xi\left(\frac{h_{j+1,n+\frac{1}{2}} - h_{j,n+\frac{1}{2}}}{\Delta\xi}\right)\right.$$
$$\left. + j\Delta\xi\left(\frac{h_{j,n+\frac{1}{2}} - h_{j-1,n+\frac{1}{2}}}{\Delta\xi}\right)\right] \tag{3.12}$$
$$d_{n+\frac{1}{2}} = 1 - 2r_{n+\frac{1}{2}}\left(\frac{\mathrm{d}r}{\mathrm{d}t}\right)_{n+\frac{1}{2}}(n+\tfrac{1}{2})\Delta\tau \tag{3.13}$$
$$k_{j+\frac{1}{2},n+\frac{1}{2}} = \frac{\rho g}{3\mu}\left(\frac{h_{j,n+\frac{1}{2}} + h_{j+1,n+\frac{1}{2}}}{2}\right)^3 \tag{3.14}$$
$$k_{j-\frac{1}{2},n+\frac{1}{2}} = \frac{\rho g}{3\mu}\left(\frac{h_{j-1,n+\frac{1}{2}} + h_{j,n+\frac{1}{2}}}{2}\right)^3 \tag{3.15}$$

Obviously, we can recombine some terms:

$$h_{j,n+1} - h_{j,n} = \frac{\Delta\tau}{(j+\frac{1}{2})d_{n+\frac{1}{2}}\Delta\xi^2}\left\{jk_{j-\frac{1}{2}}p_{j-1} - [jk_{j-\frac{1}{2}} + (j+1)k_{j+\frac{1}{2}}]p_j + (j+1)k_{j+\frac{1}{2}}p_{j+1}\right\}_{n+\frac{1}{2}}$$
$$p_j(\tau) = h_j - \frac{\lambda^2}{(j+\frac{1}{2})r^2\Delta\xi^2}[jh_{j-1} - (2j+1)h_j + (j+1)h_{j+1}] \tag{3.16}$$

Now, we replace $\vec{p}_{n+\frac{1}{2}}$ with the average of the values of t_n and t_{n+1},

$$p_{j,n+\frac{1}{2}} = \frac{p_{j,n+1} + p_{j,n}}{2}$$

so that we obtain a difference equation of Crank-Nicholson type:

$$h_{j,n+1} - \frac{\Delta\tau}{(j+\frac{1}{2})d_{n+\frac{1}{2}}\Delta\xi^2}\left\{jk_{j-\frac{1}{2},n+\frac{1}{2}}p_{j-1,n+1} - [jk_{j-\frac{1}{2},n+\frac{1}{2}} + (j+1)k_{j+\frac{1}{2},n+\frac{1}{2}}]p_{j,n+1} + (j+1)k_{j+\frac{1}{2}}p_{j+1,n+1}\right\}$$
$$= h_{j,n} - \frac{\Delta\tau}{(j+\frac{1}{2})d_{n+\frac{1}{2}}\Delta\xi^2}\left\{jk_{j-\frac{1}{2},n+\frac{1}{2}}p_{j-1,n} - [jk_{j-\frac{1}{2},n+\frac{1}{2}} + (j+1)k_{j+\frac{1}{2},n+\frac{1}{2}}]p_{j,n} + (j+1)k_{j+\frac{1}{2},n+\frac{1}{2}}p_{j+1,n}\right\} \tag{3.17}$$

We may re-express the Crank-Nicholson equation as a pentadiagonal system for $\vec{h}_{n+1}$:

$$h_{j,n+1} - \frac{2\Delta\tau}{(2j+1)d_{n+\frac{1}{2}}\Delta\xi^2}\sum_{k=-2}^{2} a_{j+k,n+\frac{1}{2}}h_{j+k,n+1} = h_{j,n} + \frac{2\Delta\tau}{(2j+1)d_{n+\frac{1}{2}}\Delta\xi^2}\sum_{k=-2}^{2} a_{j+k,n+\frac{1}{2}}h_{j+k,n} \tag{3.18}$$

where the coefficients are given by

$$a_{j-2,n+\frac{1}{2}} = -\left[\frac{j-1}{2j-1}\frac{2\lambda^2}{r_{n+\frac{1}{2}}^2\Delta\xi^2}\right] jk_{j-\frac{1}{2},n+\frac{1}{2}} \tag{3.19}$$

$$a_{j-1,n+\frac{1}{2}} = \left[1+\frac{3j+1}{2j+1}\frac{2\lambda^2}{r_{n+\frac{1}{2}}^2\Delta\xi^2}\right] jk_{j-\frac{1}{2},n+\frac{1}{2}} + \left[\frac{j}{2j+1}\frac{2\lambda^2}{r_{n+\frac{1}{2}}^2\Delta\xi^2}\right](j+1)k_{j+\frac{1}{2},n+\frac{1}{2}} \tag{3.20}$$

$$a_{j,n+\frac{1}{2}} = -\left[1+\frac{3j-1}{2j-1}\frac{2\lambda^2}{r_{n+\frac{1}{2}}^2\Delta\xi^2}\right] jk_{j-\frac{1}{2},n+\frac{1}{2}} - \left[1+\frac{3j+4}{2j+3}\frac{2\lambda^2}{r_{n+\frac{1}{2}}^2\Delta\xi^2}\right](j+1)k_{j+\frac{1}{2},n+\frac{1}{2}} \tag{3.21}$$

$$a_{j+1,n+\frac{1}{2}} = \left[\frac{j+1}{2j+1}\frac{2\lambda^2}{r_{n+\frac{1}{2}}^2\Delta\xi^2}\right] jk_{j-\frac{1}{2},n+\frac{1}{2}} + \left[1+\frac{3j+2}{2j+1}\frac{2\lambda^2}{r_{n+\frac{1}{2}}^2\Delta\xi^2}\right](j+1)k_{j+\frac{1}{2},n+\frac{1}{2}} \tag{3.22}$$

$$a_{j+2,n+\frac{1}{2}} = -\left[\frac{j+2}{2j+3}\frac{2\lambda^2}{r_{n+\frac{1}{2}}^2\Delta\xi^2}\right](j+1)k_{j+\frac{1}{2},n+\frac{1}{2}} \tag{3.23}$$

(derivation commented out; doesn't hurt to double check these coefficients).

Note that if $\lambda = 0$ (no surface tension), then the problem reduces to a tridiagonal system.

3.3 Difference equations near the boundaries

Special attention needs to be given to the equations near the center and rim of the drop.

3.3.1 $j = 0$

We have $h_{-1}(\tau) = h_0(\tau)$ and $p_{-1}(\tau) = p_0(\tau)$. We can simply set $k_{j-\frac{1}{2},n+\frac{1}{2}} = 0$ in order to satisfy the second condition, then combine a_{j-1} and a_j to satisfy the second condition.

3.3.2 $j = 1$

We have $h_{-1}(\tau) = h_0(\tau)$. Simply combine a_{j-2} and a_{j-1} to satisfy this condition.

3.3.3 $j = J-3$

We have $h_{J-1}(\tau) = h^* - \alpha r_n\Delta\xi/2$. Simply move the term multiplying a_{j+2} to the right-hand side of the equation.

3.3.4 $j = J-2$

We have $h_{J-1}(\tau) = h^* - \alpha r_n\Delta\xi/2$ and $h_J(\tau) = h^* + \alpha r_n\Delta\xi/2$. Simply move the terms multiplying a_{j+1} and a_{j+2} to the right-hand side of the equation.

4 Algorithm

Let's keep t as is, only redefine $\sigma \to \xi$. Thus, replace $d_{n+\frac{1}{2}}$ with $r^2_{n+\frac{1}{2}}$ in the above equations.

1. (Initialization) Set $n = 0$ and $\vec{h}_n = \vec{h}_0$ (initial condition).

2. (Prediction) Given $\vec{h}_n$, $\vec{\nu} = [\mu/(\rho g), \lambda, h^*, \alpha, \Omega]$, Δt, $\Delta\xi$. Set $\Delta t' = \Delta t/2$, $\vec{h}' = \vec{h}_n$. Compute the drop radius,

$$r = \left[\frac{\Omega}{\pi \Delta\xi^2 \left[J h^* + \sum_{j=1}^{J-1} j(h'_{j-1} + h'_j) \right]} \right]^{\frac{1}{2}}$$

   the coefficients,

$$T = \frac{2\Delta t'}{r^2 \Delta\xi^2}, \qquad S = \frac{2\lambda^2}{r^2\Delta\xi^2}, \qquad R = \frac{\alpha r \Delta\xi}{2}$$

   and, finally, the diffusion coefficients,

$$k_{j+\frac{1}{2}} = \frac{\rho g}{3\mu} \left(\frac{h'_j + h'_{j+1}}{2} \right)^3, \qquad k_{j-\frac{1}{2}} = \frac{\rho g}{3\mu} \left(\frac{h'_{j-1} + h'_j}{2} \right)^3, \qquad j = 0, 1, \ldots, J-2$$

   Project $\vec{h}$ to $t_{n+\frac{1}{2}}$ using a centered Taylor series projection. That is, set $\vec{v} = \vec{h}_n$ and solve the pentadiagonal system,

$$u_j - \frac{T}{2j+1} \sum_{k=-2}^{2} a_{j+k} u_{j+k} = v_j + \frac{T}{2j+1} \left(f_j + \sum_{k=-2}^{2} a_{j+k} v_{j+k} \right)$$

   where the coefficients a_{j+k} and f_j are given below. Then, set $\vec{h}_{n+\frac{1}{2}} = \vec{u}$.

3. (Correction) Now set $\Delta t' = \Delta t$ and $\vec{h}' = \vec{h}_{n+\frac{1}{2}}$. Recompute r, T, S, R, and k as defined above using these new parameters. Then, solve the pentadiagonal system above with $\vec{v} = \vec{h}_n$. Set $\vec{h}_{n+1} = \vec{u}$.

4. (Recursion) Advance n by 1 and repeat steps 2 and 3.

4.1 Pentadiagonal coefficients

4.1.1 $2 \le j \le J-4$

$$a_{j-2} = -S\left(\frac{j-1}{2j-1}\right) jk_{j-\frac{1}{2}} \tag{4.1}$$

$$a_{j-1} = \left[1 + S\left(\frac{3j+1}{2j+1}\right)\right] jk_{j-\frac{1}{2}} + S\left(\frac{j}{2j+1}\right)(j+1)k_{j+\frac{1}{2}} \tag{4.2}$$

$$a_j = -\left[1 + S\left(\frac{3j-1}{2j-1}\right)\right] jk_{j-\frac{1}{2}} - \left[1 + S\left(\frac{3j+4}{2j+3}\right)\right](j+1)k_{j+\frac{1}{2}} \tag{4.3}$$

$$a_{j+1} = S\left(\frac{j+1}{2j+1}\right) jk_{j-\frac{1}{2}} + \left[1 + S\left(\frac{3j+2}{2j+1}\right)\right](j+1)k_{j+\frac{1}{2}} \tag{4.4}$$

$$a_{j+2} = -S\left(\frac{j+2}{2j+3}\right)(j+1)k_{j+\frac{1}{2}} \tag{4.5}$$

$$f_j = 0 \tag{4.6}$$

4.1.2 $j = 0$

$$a_{j-2} = 0 \tag{4.7}$$

$$a_{j-1} = 0 \tag{4.8}$$

$$a_j = -\left[1 + S\left(\frac{3j+4}{2j+3} - \frac{j}{2j+1}\right)\right](j+1)k_{j+\frac{1}{2}} \tag{4.9}$$

$$a_{j+1} = \left[1 + S\left(\frac{3j+2}{2j+1}\right)\right](j+1)k_{j+\frac{1}{2}} \tag{4.10}$$

$$a_{j+2} = -S\left(\frac{j+2}{2j+3}\right)(j+1)k_{j+\frac{1}{2}} \tag{4.11}$$

$$f_j = 0 \tag{4.12}$$

4.1.3 $j = 1$

$$a_{j-2} = 0 \tag{4.13}$$

$$a_{j-1} = \left[1 + S\left(\frac{3j+1}{2j+1} - \frac{j-1}{2j-1}\right)\right] jk_{j-\frac{1}{2}} + S\left(\frac{j}{2j+1}\right)(j+1)k_{j+\frac{1}{2}} \tag{4.14}$$

$$a_j = -\left[1 + S\left(\frac{3j-1}{2j-1}\right)\right] jk_{j-\frac{1}{2}} - \left[1 + S\left(\frac{3j+4}{2j+3}\right)\right](j+1)k_{j+\frac{1}{2}} \tag{4.15}$$

$$a_{j+1} = S\left(\frac{j+1}{2j+1}\right) jk_{j-\frac{1}{2}} + \left[1 + S\left(\frac{3j+2}{2j+1}\right)\right](j+1)k_{j+\frac{1}{2}} \tag{4.16}$$

$$a_{j+2} = -S\left(\frac{j+2}{2j+3}\right)(j+1)k_{j+\frac{1}{2}} \tag{4.17}$$

$$f_j = 0 \tag{4.18}$$

4.1.4 $j = J - 3$

$$a_{j-2} = -S\left(\frac{j-1}{2j-1}\right) jk_{j-\frac{1}{2}} \tag{4.19}$$

$$a_{j-1} = \left[1 + S\left(\frac{3j+1}{2j+1}\right)\right] jk_{j-\frac{1}{2}} + S\left(\frac{j}{2j+1}\right)(j+1)k_{j+\frac{1}{2}} \tag{4.20}$$

$$a_j = -\left[1 + S\left(\frac{3j-1}{2j-1}\right)\right] jk_{j-\frac{1}{2}} - \left[1 + S\left(\frac{3j+4}{2j+3}\right)\right](j+1)k_{j+\frac{1}{2}} \tag{4.21}$$

$$a_{j+1} = S\left(\frac{j+1}{2j+1}\right) jk_{j-\frac{1}{2}} + \left[1 + S\left(\frac{3j+2}{2j+1}\right)\right](j+1)k_{j+\frac{1}{2}} \tag{4.22}$$

$$a_{j+2} = 0 \tag{4.23}$$

$$f_j = -2\left(h^* + R\right) S\left(\frac{j+2}{2j+3}\right)(j+1)k_{j+\frac{1}{2}} \tag{4.24}$$

4.1.5 $j = J - 2$

$$a_{j-2} = -S\left(\frac{j-1}{2j-1}\right) jk_{j-\frac{1}{2}} \tag{4.25}$$

$$a_{j-1} = \left[1 + S\left(\frac{3j+1}{2j+1}\right)\right] jk_{j-\frac{1}{2}} + S\left(\frac{j}{2j+1}\right)(j+1)k_{j+\frac{1}{2}} \tag{4.26}$$

$$a_j = -\left[1 + S\left(\frac{3j-1}{2j-1}\right)\right] jk_{j-\frac{1}{2}} - \left[1 + S\left(\frac{3j+4}{2j+3}\right)\right](j+1)k_{j+\frac{1}{2}} \tag{4.27}$$

$$a_{j+1} = 0 \tag{4.28}$$

$$a_{j+2} = 0 \tag{4.29}$$

$$\begin{aligned} f_j = &-2\left(h^* - R\right) S\left(\frac{j+2}{2j+3}\right)(j+1)k_{j+\frac{1}{2}} \\ &+ 2(h^* + R)\left\{S\left(\frac{j+1}{2j+1}\right) jk_{j-\frac{1}{2}} + \left[1 + S\left(\frac{3j+2}{2j+1}\right)\right](j+1)k_{j+\frac{1}{2}}\right\} \end{aligned} \tag{4.30}$$