

Appendix D. Numerical methods

D.1. Numerical solution of rim equation

Here, we describe our numerical method for solving the boundary value problem for the rim profile, defined by equations (3.9), (3.10), and (4.13). For a fixed value of the parameter q , equations (3.9) and (4.13) were recast as

$$\frac{d^3 \tilde{h}^{(n+1)}(\tilde{x})}{d\tilde{x}^3} = \frac{q}{\tilde{h}^{(n)}(\tilde{x})} \frac{2}{\pi} \int_{-\infty}^{\infty} \log |\tilde{x} - \tilde{y}| \frac{d^2}{d\tilde{y}^2} \left(1/\tilde{h}^{(n)}(\tilde{x}) \right) d\tilde{y}, \quad (\text{D } 1)$$

with boundary conditions

$$\tilde{h}^{(n+1)}(0) = 1, \quad \left. \frac{d\tilde{h}^{(n+1)}(\tilde{x})}{d\tilde{x}} \right|_{\tilde{x}=0} = 0, \quad \left. \frac{d^2 \tilde{h}^{(n+1)}(\tilde{x})}{d\tilde{x}^2} \right|_{\tilde{x}=0} = 1. \quad (\text{D } 2)$$

Boundary condition (3.10) was enforced by rescaling \tilde{x} after the converged profile $\tilde{h}(\tilde{x})$ is obtained.

Equations (D 1) and (D 2) were solved by iteration, where $\tilde{h}^{(n+1)}(\tilde{x})$ is the profile corresponding to $n + 1$ iterations, and $\tilde{h}^{(0)}(\tilde{x}) = \tilde{x}^2$. The transformation (D 1) and (D 2) is a contracting map; we observed that $\tilde{h}^{(n)}(\tilde{x})$ converges exponentially to a fixed point $\tilde{h}(\tilde{x})$. The convergence exponent vanishes for $q \rightarrow q^*$, and we were unable to obtain a solution for $q > q^*$, indicating that $q = q^*$ is a turning point. Solutions corresponding to $q > q^*$ collapse at a finite negative value of \tilde{x} and are thus unphysical.

The critical parameter value (4.16) was obtained by advancing the parameter q using interval halving. The coefficient (4.18) of the square-root far-field film profile (4.17) was extracted from the profile corresponding to $q = q^*$.

The iterative solution was obtained on the finite computational domain, $-X_1 < x < X_2$, using approximations for the tails of the integral in equation (D 1), $x > X_2$ and $x < -X_1$, based on the asymptotic far-field forms (3.10) and (4.17). The cut-off parameters X_1 and X_2 were increased starting with an iterative solution for modest values of these parameters, until convergent results were obtained.

D.2. Numerical solution of dome equation

Integral equation (5.24) was solved using a Galerkin formulation, in which the L_2 norm of the residual was minimized as a functional of $D_2[\bar{\omega}_d](r)$. By symmetry, the film profile has an expansion in even powers of r about $r = 0$ as does the velocity profile $\bar{\omega}_d(r)$, but $D_2[\bar{\omega}_d](r)$ has an odd-power expansion about $r = 0$. At the edge of the dome region, $D_2[\bar{\omega}_d](r)$ has the singular behavior (5.14). Based on the form of $D_2[\bar{\omega}_d](r)$ for $r \rightarrow 0$ and $r \rightarrow 1^-$, the function $D_2[\bar{\omega}_d](r)$ was represented in terms of basis functions given by

$$D_2[\bar{\omega}_d](r) = \sum_{k=0}^N a_k r(1-r^2)^{k-5/2}, \quad (\text{D } 3)$$

where a_k ($k = 0, 1, 2, \dots$) are the expansion coefficients. Our numerical solution of equation (5.24) was insensitive to the form of the basis functions; the same results were obtained with other basis functions that have the proper symmetry at $r = 0$ and proper singular behavior at $r = 1$.

After solving equation (5.24) for $D_2[\bar{\omega}_d](r)$, as described above, the velocity profile was obtained by integrating equation (5.9) from $r = 0$ using initial conditions compatible with equation (5.4):

$$\bar{\omega}_d(r) = \frac{1}{2} \int_0^r (r^2 - R^2) D_2[\bar{\omega}_d] dR + \frac{1}{2} r^2. \quad (\text{D } 4)$$

The volume profile $\bar{\Omega}(r)$ and the film thickness $\bar{h}_d(r)$ were derived from $\bar{\omega}_d(r)$ using equations (5.27)–(5.28).

Inserting the basis-function expansion (D 3) into equation (5.14) yields the amplitude of the square-root film profile at the rim (5.11),

$$\bar{\alpha} = 3\sqrt{2}a_0^{-1}\bar{\Omega}_1, \quad (\text{D } 5)$$

where a_0 is the first expansion coefficient in (D 3) and $\bar{\Omega}_1$ is the dome volume. According to our numerical solution, $a_0 \doteq 1.500$ and $\bar{\Omega}_1$ is given by (5.31), thus we obtain the numerical value of $\bar{\alpha}$ by equation (5.32).

D.3. *Discretization for thin film simulations*

In our thin film simulations, the interface was discretized on the finite interval $0 \leq r \leq R_\infty$ (where R_∞ is a cutoff parameter). To resolve the lateral length scales in the rim as well as in the dome and outer regions the spatial coordinate r was discretized using non-uniform adaptive mesh, defined by the time-dependent mesh-point density function

$$\rho(r, t) = N_0 [(1 - x_r)R_\infty^{-1} + x_r g(\tilde{x})]. \quad (\text{D } 6)$$

Here, N_0 is the number of mesh points, x_r is the fraction of mesh points used to discretize the rim region, $g(\tilde{x})$ is a normalized distribution function that resolves the curvature, curvature gradient, and tangential stress in the rim region, and \tilde{x} is the rim variable (3.6). Accurate resolution of the far-field rim stress was found to be important, thus a distribution function with algebraic decay compatible with equation (4.19) was used in our simulations. Given the normalization $\int_{-\infty}^{+\infty} g(t)dt = 1$, the node-point density function (D 6) satisfies $\int_0^{R_\infty} \rho(r, t) dr = N_0$ at long times, $h_m^{-1/2}(t) \gg 1$.

In our simulations, approximately two-thirds of the nodes were used to resolve the rim region, i.e., $x_r \approx 2/3$. Our long-time numerical results were insensitive to the truncation in r for $R_\infty > 3$; however, we used $R_\infty = 20$ in order to resolve the short-time behavior also. For x_r and R_∞ fixed, we observed $O(N_0^{-2})$ numerical convergence. The results depicted in figures 6–9 were obtained using $N_0 = 300$ and are converged to the resolution of the figures.