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Continuation

THFI : Sliding drops modelled by a thin film equation for a liquid layer or drop on an inclined homogeneous substrate

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www.uni-muenster.de/CeNoS/Lehre/Tutorials/auto.html

2 thfi : Sliding drops modelled by a thin film equation for a liquid layer or drop on an inclined homogeneous substrate

In the tutorial THFI a dimensionless thin film equation closely related to the one in DROP is used. In this case a lateral driving force is included and solutions for sliding drops on an inclined plane are examined. You will calculate steady solutions [in the comoving frame], in particular, drops moving at a constant velocity. The main treated control parameter is the inclination angle.

2.1 Model

This demo illustrates the calculation of sliding drop and surface wave solutions of the dimensionless thin film equation

$$\partial_t h = -\partial_x \{Q(h)\,\partial_x\,[\partial_{xx}h - \partial_h f(h)] + \chi(h)\} \tag{2.1}$$

where $Q(h) = h^3$ is the mobility function and $\chi(h)$ is the lateral driving. For an inclined substrate it is $\chi = \alpha Q(h)$ with α being the inclination angle. For background information see [1, 2]. Examples of similar calculations with various $f(h)$ can be found in [3, 4, 5]. The term in square brackets corresponds to a pressure. The pressure used here is the same as in the demo `drop` [6] where it is explained in detail. Our aim is to study sliding droplet or surface wave

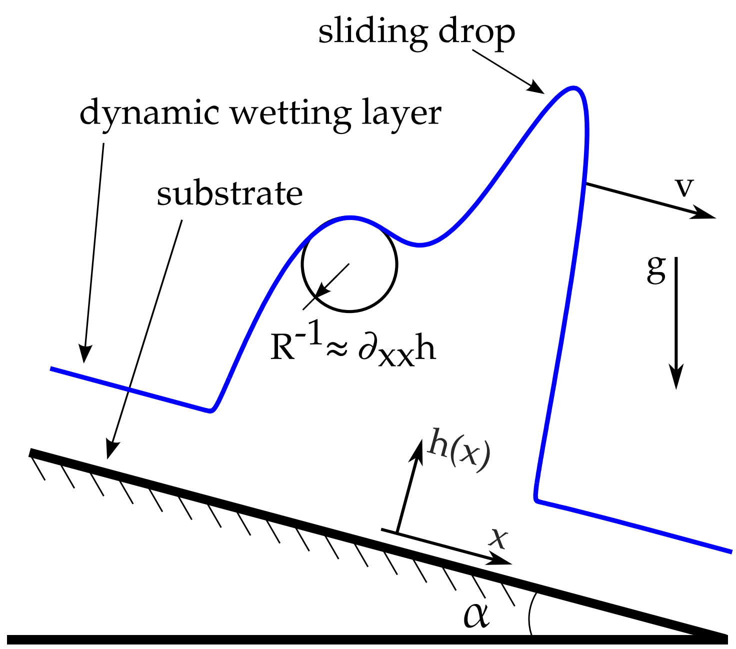

Figure 2.1: The basic geometry for this problem. The profile is an actual solution to the equation of this problem.

solutions that are steady in some co-moving frame, i.e., the drops slide with constant speed v and shape. We introduce the coordinate in the frame moving with v by $\tilde{x} = x - vt$ and obtain from Eq. (2.1) after dropping the tildes

$$-v\partial_x h = -\partial_x \{Q(h)\,\partial_x\,[\partial_{xx}h - \partial_h f(h)] + \chi(h)\} \tag{2.2}$$

Eq. (2.2) is integrated once to obtain

$$0 = Q(h)\,\partial_x\left[\partial_{xx}h - \partial_h f(h)\right] + \chi(h) - vh - C_0 \tag{2.3}$$

where the constant C_0 corresponds to the flux in the co-moving frame and the unknown velocity v can be seen as an eigenvalue in a nonlinear eigenvalue problem. Note that $C_0 + vh$ is the flux in the laboratory frame.

To use the continuation toolbox auto07p [7], we first write (2.3) as a system of first-order autonomous ordinary differential equations on the interval $[0, 1]$. Therefore, we introduce the variables $u_1 = h - h_0$, $u_2 = dh/dx$ and $u_2 = d^2h/dx^2$, use $\chi(h) = \alpha Q(h)$, and obtain from equation (2.3) the 3d dynamical system (NDIM $= 3$)

$$\begin{aligned} \dot{u}_1 &= Lu_2 \\ \dot{u}_2 &= Lu_3 \\ \dot{u}_3 &= L\left[u_2 f''(u_1 + h_0) - \alpha + \tfrac{v(u_1+h_0)+C_0}{Q(u_1+h_0)}\right]. \end{aligned} \tag{2.4}$$

where L is the physical domain size, and dots and primes denote derivatives with respect to $\xi \equiv x/L$ and h, respectively. The advantage of the used form is that the fields $u_1(\xi)$, $u_2(\xi)$ and $u_3(\xi)$ correspond to the correctly scaled physical fields $h(L\xi)$, $\partial_x h(L\xi)$ and $\partial_{xx}h(L\xi)$. We use periodic boundary conditions for all u_i (NBC $= 3$) that take the form

$$u_1(0) = u_1(1), \tag{2.5}$$
$$u_2(0) = u_2(1), \tag{2.6}$$
$$u_3(0) = u_3(1), \tag{2.7}$$

and integral conditions for mass conservation and computational pinning (to break the translational symmetry that the solutions have on the considered homogeneous substrate) (NINT $= 2$). The integral condition for mass conservation takes the form

$$\int_0^1 u_1\,\mathrm{d}\xi = 0. \tag{2.8}$$

There are two ways to start the continuation. Either (i) one sets $\alpha = 0$ and uses as in the demo `drop` [6] the starting solution consisting of small amplitude harmonic modulation of wavelength $L_c = 2\pi/k_c$ where $k_c = \sqrt{-f''(h_0)}$ is the critical wavenumber for the linear instability of a flat film of thickness h_0 and also sets initially $v = 0$ and $C_0 = 0$; or (ii) one starts at some $\alpha \neq 0$, uses small amplitude harmonic starting solution with $L_c = 2\pi/k_c$ and initialises $v = \alpha Q'(h_0)$ and $C_0 = \alpha Q(h_0) - vh_0$. In the present demo we use the former option.

The number of free (continuation) parameters is given by NCONT $=$ NBC$+$NINT$-$NDIM$+1$ and is here equal to 3. For more details see [2].

2.2 Runs:

Python interface command line	**Terminal command line**
auto	
run 1: Determine steady solutions on the horizontal substrate as a function of domain size L, starting at the critical L_c with a small amplitude sinusoidal solution. Mean thickness is fixed. Compute the branch of periodic solutions for $h_0 = 5$ continued in L (PAR(5)) up to $L = 400$. **Remaining true continuation parameters:** C_0 (PAR(6)) and v (PAR(42)); **Parameters:** IPS$=4$, ISP$=0$, ISW$=1$, ICP$=[5,6,42]$, Start data from function *stpnt* (IRS$=0$) save output-files as `b.d1, s.d1, d.d1`	
r1 = run(e = 'thfi', c = 'thfi.1', sv = 'tf1')	*@@R thfi 1* *@sv tf1*
run 11: Restart at domain size $L = 400$, keep mean thickness h_0 fixed and incline substrate to observe transition from sliding drops to surface waves. Continued in inclination α (PAR(41)) for fixed domain size L. Stop at $\alpha = 0.01$ **Remaining true continuation parameters:** C_0 (PAR(6)) and and v (PAR(42)); **Other output:** abs. value of minimal slope of h (PAR(46)), i.e., advancing dynamic contact angle $\theta_{\rm adv}$; maximal slope of h (PAR(47)), i.e., receding dynamic contact angle $\theta_{\rm rec}$; **Parameter:** IPS$=4$, ISP$=0$, ISW$=1$, ICP$=[41,6,42,46,47]$, Start at final result of run 1: IRS$=7$ save output-files as `b.d11, s.d11, d.d11`	
r11 = run(r1, e = 'thfi', c = 'thfi.11', sv = 'thfi11')	*@@R thfi 11 tf1* *@sv tf11*
clean()	*@cl*

Table 2.1: Commands for running demo `thfi`.

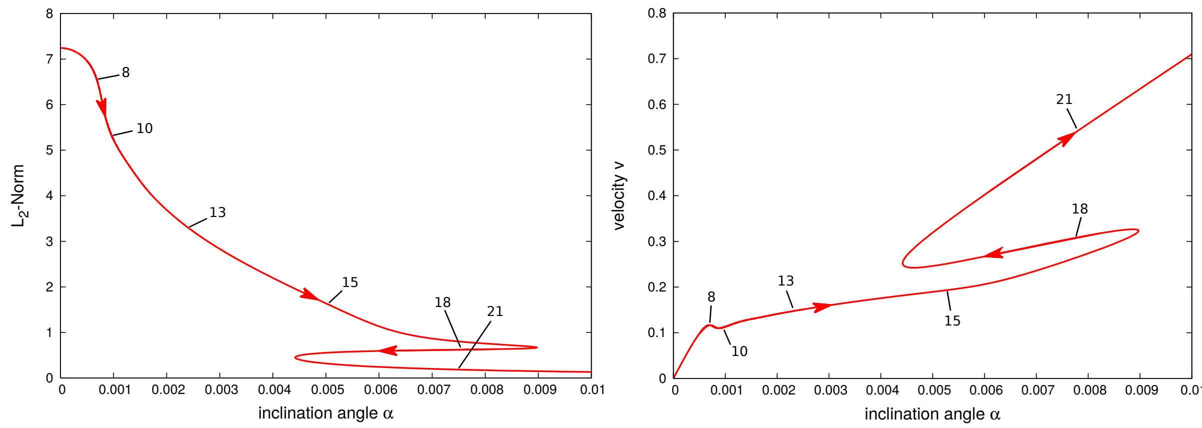

Figure 2.2: An illustration for run 11 of demo `thfi` is given. The L_2-norm of stationary solutions (steady in the frame moving with v) is shown in dependence of the principal continuation parameter inclination angle α (par(41)) for fixed domain size $L = 400$ (par(5)) and mean thickness $h_0 = 5$ (par(1)).

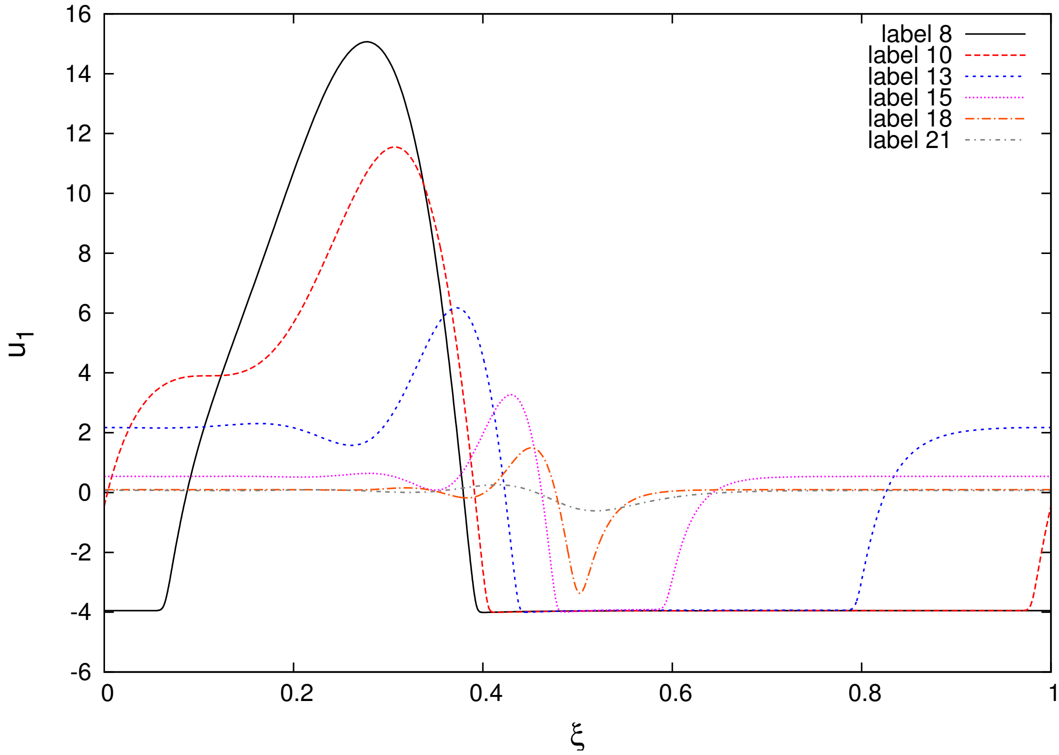

Figure 2.3: Stationary film thickness profiles corresponding to Fig. (2.2) at inclination angles as given in the legend. The profiles are represented by $u_1(\xi) = h(\xi L) - h_0$ where $h_0 = 5$.

2.3 Remarks:

- Beside the NCONT true continuation parameters that have to be given as ICP in the c.* parameter file, one may list other output parameters as defined in the subroutine PVLS in the *.f90 file.
- As in the demo `drop` [6] one may define other integral conditions to determine integral measures one might be interested in
- Screen output and command line commands are provided in README file.

2.4 Tasks:

After running the examples, you should try to implement your own adaptations, e.g.:

1. Redo runs 1 and 11 for other values of h_0.
2. Try to run instead of run 11 a continuation with fixed C_0. You need to 'set free' another parameter. This will not work if $\alpha = 0$ initially. Start from a solution of the original run 11.
3. Include additional integral condition(s), to measure characteristics of interest. These might be the surface energy, wetting energy, total energy dissipation.

4. Replace the used Derjaguin pressure by a different one that you get from the literature.
5. Replace the used mobility function $Q(h)$ by a different one. An option is $Q = h^2(h + l_s)/3\eta$ that incorporates slip of the liquid at the solid substrate (l_s is the slip length).

References

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