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# Continuation

## HETDROP : Steady states of a thin film equation for a liquid layer or drop on a horizontal heterogeneous substrate

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# 3 hetdrop : Steady states of a thin film equation for a liquid layer or drop on a horizontal heterogeneous substrate

In the tutorial HETDROP the dimensionless thin film equation used in the tutorial DROP is adapted to a substrate of varying wettability. In particular, the long-range contribution of the disjoining pressure is sinodally modulated. You will calculate steady solutions and their bifurcations that emerge when using the heterogeneity strength as control parameter.

## 3.1 Model

This demo illustrates the calculation of steady drop and hole solutions of the dimensionless thin film equation

$$\partial_t h \;=\; -\partial_x \left\{Q(h)\,\partial_x \left[\partial_{xx}h - \partial_h f(h,x)\right]\right\} \tag{3.1}$$

For an explanation of the basic structure of the equation see demo `drop` [1]. The only difference to the demo `drop` is that the Derjaguin pressure $-\partial_h f(h,x)$ now depends explicitly on position $x$, i.e., we have a substrate that has a non-constant wettability. Such a system was studied in [2] and in the first part of [3]. Here we assume a sinusoidal modulation of the long range contribution to the pressure:

$$\partial_h f(h,x) = -\Pi(h) = \frac{1}{h^3}\left[1+\rho\sin(2\pi x/P)\right] - \frac{1}{h^6}. \tag{3.2}$$

where $\rho$ and $P$ are the relative strength and period of the heterogeneity. Note that the domain size $L$ and the period of the heterogeneity are normally not identical. In a periodic setting one has $L = nP$ where $n > 0$ is an integer.

To study steady solutions, i.e., resting droplets or films, we set as in the demo `drop` [1] $\partial_t h = 0$ and integrate Eq. (1.1) twice to obtain

$$0 \;=\; \partial_{xx}h(x) \;-\; \partial_h f(h,x) \;+\; C_1. \tag{3.3}$$

Here the constant $C_1$ takes the role of a Lagrange multiplier for mass conservation.

When writing Eq. (3.3) as a system of first-order ordinary differential equations on the interval $[0,\,1]$ (introducing $u_1 = h - h_0$ and $u_2 = dh/dx$) we obtain the non-autonomous system (r.h.s depends explicitly on $x$)

$$\begin{aligned} \dot{u}_1 &= L u_2 \\ \dot{u}_2 &= L\left[\partial_h f(h_0+u_1,x) \;-\; C_1\right]. \end{aligned} \tag{3.4}$$

where $L$ is the physical domain size, and dots indicate derivatives with respect to $\xi \equiv x/L$, and $f_h$ is the partial derivative of $f$ w.r.t. $h$. Such a non-autonomous system can not be handled by auto07p [4], therefore we need to transform it into an autonomous one. This is done by defining the position variable $x$ to be a third independent variable, i.e., $u_3 = x$ that as the other $u_i$ depends on the independent variable $\xi$. One obtains the 3d dynamical system ($\mathrm{NDIM} = 3$)

$$\begin{aligned} \dot{u}_1 &= L u_2 - \epsilon[\partial_{u_1} f(h_0+u_1,u_3) \;-\; C_1] \\ \dot{u}_2 &= L\left[\partial_{u_1} f(h_0+u_1,u_3) \;-\; C_1\right] \\ \dot{u}_3 &= L. \end{aligned} \tag{3.5}$$

We use periodic boundary conditions for $u_1$ and $u_2$ that take the form

$$u_1(0) = u_1(1), \tag{3.6}$$
$$u_2(0) = u_2(1), \tag{3.7}$$
$$\tag{3.8}$$

as 3rd BC we 'pin' the physical position $x$ to computational one by

$$u_3(0) = 0, \tag{3.9}$$

i.e., $\mathrm{NBC} = 3$). We also use an integral condition for mass conservation ($\mathrm{NINT} = 1$) that takes the form

$$\int_0^1 u_1 \, \mathrm{d}\xi = 0. \tag{3.10}$$

As starting solution we use a flat film of height $h_0$, i.e., $u_1 = u_2 = 0$, fix the domain size $L$ and set $u_3 = L\xi$ and $\rho = 0$. The starting value for $C_1$ is $\partial_{u_1} f(h_0, u_3)$ at $\rho = 0$, i.e., the $x$-independent $f'(h_0)$.

The number of free (continuation) parameters is given by $\mathrm{NCONT} = \mathrm{NBC}+\mathrm{NINT}-\mathrm{NDIM}+1$ and is here equal to 2.

Note that in Eq. (3.5) we keep the term with the unfolding parameter $\epsilon$ that is explained in the demo `drop` [1]. However, in the present demo one does not need to use it if the run is done with heterogeneous substrate or uses $\rho$ as continuation parameter. However, if one wants to use the demo to look at drops on homogeneous substrate ($\rho = 0$) one might need it.

## 3.2 Runs:

| Python interface command line | Terminal command line |
|---|---|
| *auto* | |
| **run 1:** Starting with a flat film on a homogeneous substrate ($\rho = 0$), determine steady solutions as a function of heterogeneity strength $\rho$. Mean thickness $h_0 = 3$ and $L = P = 50$ is fixed (Note that $L_c \approx 33$). One finds that the branch turns at some value of $\rho$.<br>Compute the branch of periodic solutions for $h_0 = 3$ continue in heterogeneity strength $\rho$ (PAR(3)).<br>**Remaining true continuation parameters:** $C_1$ (PAR(6)), $E$ (PAR(9), we use NINT= 2)<br>**Parameters:** IPS= 4, ISP= 2, ISW= 1, ICP= $[3, 6, 9]$<br>Start data from function $stpnt$ (IRS= 0) & check that ANZ= 1 in *.f90 file.<br>Save output-files as `b.h1, s.h1, d.h1`. | |
| *r1 = run(e = 'hetdrop', c = 'hetdrop.1', sv = 'h1')* | *@@R hetdrop 1*<br>*@sv h1* |
| **run 2:** As run 1, but change to ANZ= 2 (from ANZ= 1) in *.f90 file. Beside the fold (saddle-node) now also branching points (BP) are detected.<br>Compute the branch of periodic solutions for $h_0 = 3$ continue in heterogeneity strength $\rho$ (PAR(3)).<br>**Remaining true continuation parameters:** $C_1$ (PAR(6)), $E$ (PAR(9), we use NINT= 2)<br>**Parameters:** IPS= 4, ISP= 2, ISW= 1, ICP= $[3, 6, 9]$<br>Start data from function $stpnt$ (IRS= 0) & check that ANZ= 2 in *.f90 file.<br>Save output-files as `b.h2, s.h2, d.h2`. | |
| *r2 = run(e = 'hetdrop', c = 'hetdrop.2', sv = 'h2')* | *@@R hetdrop 2*<br>*@sv h2* |
| **run 21:** Restart at BP point of run 2; switch branch and follow side branch. It shows more BPs.<br>Continue in heterogeneity strength $\rho$ (PAR(3)), branch switching (ISW= $-1$), restart at LAB12 of run 2 (IRS= 12)<br>**Remaining true continuation parameters:** $C_1$ (PAR(6))<br>**Parameters:** PS= 4, ISP= 2, ISW= $-1$, ICP= $[3, 6, 9]$.<br>Save output-files as `b.h21, s.h21, d.h21`. | |
| *r21 = run(r2, e = 'hetdrop', c = 'hetdrop.21', sv = 'h21')* | *@@R hetdrop 21 h2*<br>*@sv h21* |
| **run 211:** Restart at BP point of run 21; switch branch and follow side branch. Now one needs to look at all the obtained branches, plot norm and energy over $\rho$, look at the obtained profiles and understand the bifurcation structure.<br>Continue in heterogeneity strength $\rho$ (PAR(3)), branch switching (ISW= $-1$), restart at LAB25 of run 21 (IRS= 23)<br>**Remaining true continuation parameters:** $C_1$ (PAR(6))<br>**Parameters:** IPS= 4, ISP= 2, ISW= $-1$, ICP= $[3, 6, 9]$<br>Save output-files as `b.h211, s.h211, d.h211`. | |
| *r211 = run(r21, e = 'hetdrop', c = 'hetdrop.211', sv = 'h211')* | *@@R hetdrop 211 h21*<br>*@sv h211* |

| | |
|---|---|
| *clean()* | *@cl* |

**Table 3.1:** Commands for running demo `hetdrop`.

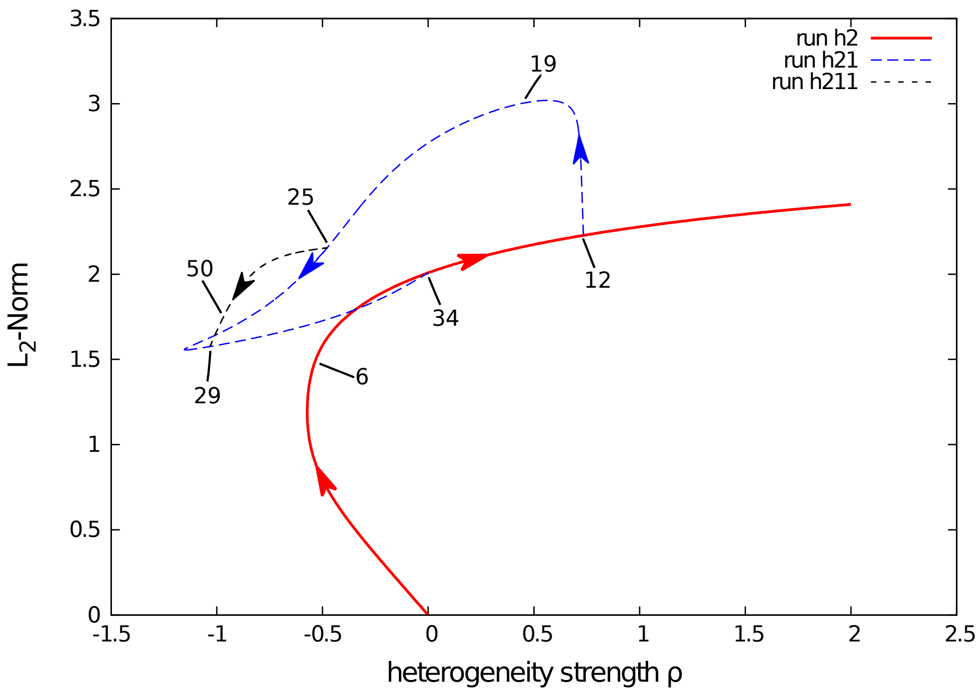


**Figure 3.1:** An illustration for runs 2, 21 and 211 (for respective linestyles see legend) of demo `hetdrop` is given. The $L_2$-norm of steady solutions is shown in dependence of the principal continuation parameterheterogeneity strength $\rho$ (par31)) for fixed domain size $L = 2P = 100$ (par(5)) and mean thickness $h_0 = 3$ (par(1)). The arrows indicates the direction of the path continuations.

## 3.3 Remarks:

- In thermodynamic context, the constant $C_1$ corresponds to the negative of the chemical potential.
- The *.f90 file provides another integral condition that is used in all runs of the demo. It allows for a determination of the energy of the obtained steady state solutions.
- As the heterogeneity profile is sinusoidal, for each solution there exists another one. It is obtained by $\rho \to -\rho$ and $h(x) \to h(x + P/2)$. I.e. when giving global measures $M(\rho)$ like norm or energy, all curves might be reflected ($M(-\rho)$) to obtain the complete picture with less calculations.
- Run 211 may not switch branches on some mashines. In that case, try changing the sign of the DS parameter in the corresponding c. file.
- Screen output and command line commands are provided in README file.

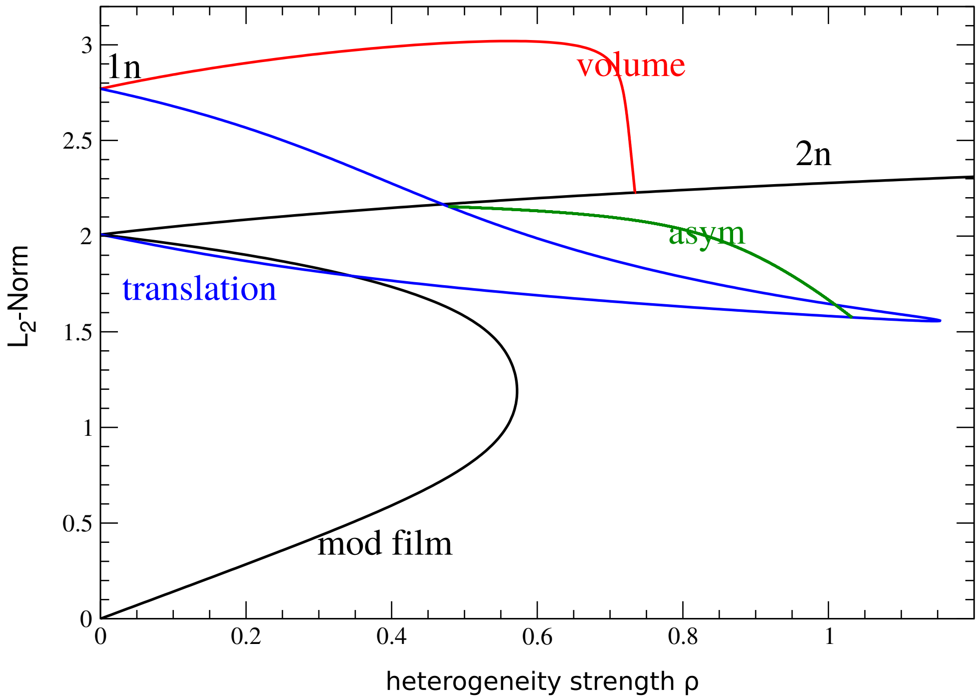


**Figure 3.2:** As equation (3.3) with (3.2) is invariant under the transformation $(\rho, x) \to (-\rho, x + P/2)$ and the used solution measures do not change under a shift in $x$, the bifurcation diagram in Fig. 3.1 is symmetric under $\rho \to -\rho$ and may therefore be completed by reflecting all curves at $\rho = 0$. The resulting complete bifurcation diagram in dependence of heterogenity strength $\rho$ (PAR(3)) is given here for $\rho \geq 0$. The various labels indicates how the branches are related.

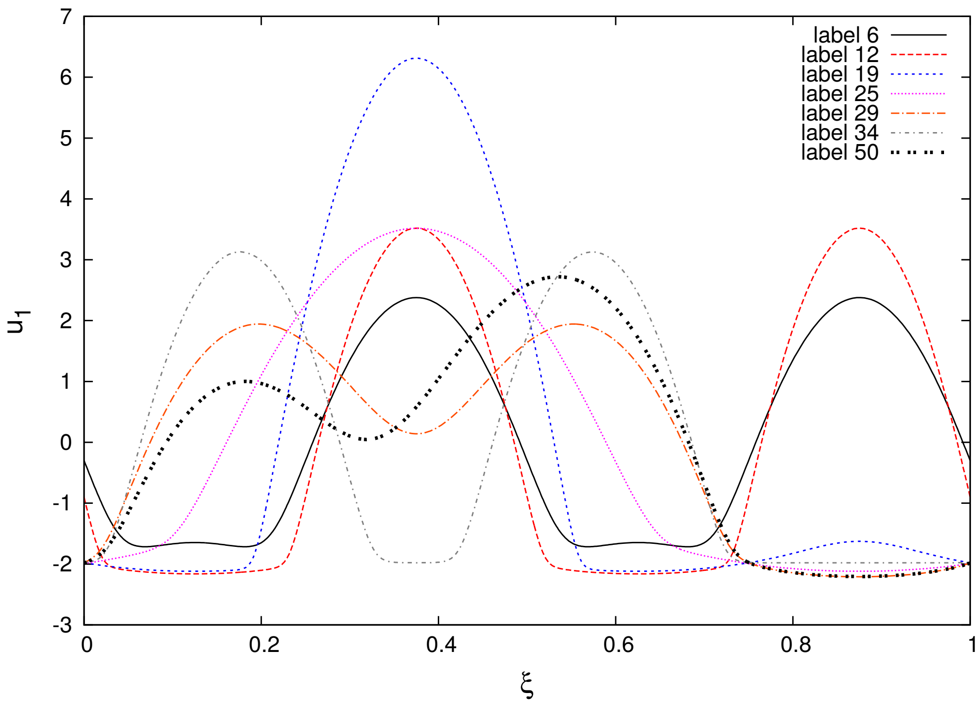


**Figure 3.3:** Steady film thickness profiles corresponding to Fig. (3.1) at heterogenity strength $\rho$ (PAR(3)) as given in the legend. The profiles are represented by $u_1(\xi) = h(\xi L) - h_0$ where $h_0 = 3$.

## 3.4 Tasks:

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

1. Redo the runs for other values of $h_0$. What do you observe?
2. Redo run 21 trying to switch branch at another label BR of run 2.
3. Try to run a continuation with fixed $C_1$ (you need to 'set free' another parameter).
4. Deactivate the integral condition that measures the energy of the solutions.
5. Modulate the short-range part of the Derjaguin pressure instead of the long-range part.
6. Replace the used Derjaguin pressure by a different one that you get from the literature.

## References

[1] U. Thiele. *Continuation tutorial: DROP*. http://www.uni-muenster.de/CeNoS/. 2014.

[2] U. Thiele et al. "Modelling thin-film dewetting on structured substrates and templates: Bifurcation analysis and numerical simulations". In: *Eur. Phys. J. E* 11 (2003), pp. 255–271. DOI: 10.1140/epje/i2003-10019-5.

[3] U. Thiele and E. Knobloch. "On the depinning of a driven drop on a heterogeneous substrate". In: *New J. Phys.* 8 (2006), p. 313. DOI: 10.1088/1367-2630/8/12/313.

[4] E.J. Doedel and B.E. Oldeman. *AUTO-07P :Continuation and bifurcation software for ordinary differential equations*. http://www.dam.brown.edu/people/sandsted/auto/auto07p.pdf. 2012.