

Münsteranian Torturials on Nonlinear Science

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Continuation

HETDROP: steady drop and film states on a horizontal heterogeneous substrate

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Abstract

The tutorial HETDROP is one of a series of tutorials on the practical application of numerical path-continuation methods for problems in soft matter and pattern formation. It is part of the “Münsteranian Torturials on Nonlinear Science”. In the tutorial the dimensionless thin-film equation used in the tutorial SITDROP [1] is adapted to a substrate with spatially varying wettability. In particular, the long-range contribution of the wetting energy is sinusoidally modulated. You will calculate steady states and their bifurcations that emerge when using the heterogeneity contrast as control parameter. The employed code package is `auto07p`. It is recommended to consider this tutorial after the tutorial SITDROP [1].

1 Model

The tutorial HETDROP is part of the “Münsteranian Torturials on Nonlinear Science”, a series of hands-on tutorials that shall facilitate the practical application of numerical path-continuation methods [2, 3, 4] for problems in soft matter and pattern formation by lowering the entrance threshold for systems where side conditions as, e.g., conservation laws and translational invariance have to be taken into account. The present tutorial is based on the code package `auto07p` [5]. An overview of all available tutorials in the series and a description of a recommended sequence of working through them is given in Ref. [6].

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

$$\partial_t h = -\partial_x \{Q(h) \partial_x [\partial_{xx} h - \partial_h f(h, x)]\} \quad (1)$$

For an explanation of the basic structure of the equation see tutorial SITDROP [1]. The only difference to the tutorial SITDROP 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 spatially modulated wettability. Such a system was studied in [7, 8] and in the first part of [9]. Here, we assume a sinusoidal modulation of the long range contribution to the pressure:

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

where ρ 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 tutorial SITDROP [1] $\partial_t h = 0$ and integrate Eq. (1) twice to obtain

$$0 = \partial_{xx} h(x) - \partial_h f(h, x) + C_1. \quad (3)$$

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

When writing Eq. (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)

$$\begin{aligned} \dot{u}_1 &= Lu_2 \\ \dot{u}_2 &= L[\partial_h f(h_0 + u_1, x) - C_1]. \end{aligned} \quad (4)$$

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 [5, 2, 10], 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 ξ . One obtains the 3d dynamical system (NDIM = 3)

$$\begin{aligned}\dot{u}_1 &= Lu_2 - \epsilon[\partial_{u_1}f(h_0 + u_1, u_3) - C_1] \\ \dot{u}_2 &= L[\partial_{u_1}f(h_0 + u_1, u_3) - C_1] \\ \dot{u}_3 &= L.\end{aligned}\tag{5}$$

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

$$u_1(0) = u_1(1),\tag{6}$$

$$u_2(0) = u_2(1),\tag{7}$$

$$\tag{8}$$

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

$$u_3(0) = 0,\tag{9}$$

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

$$\int_0^1 u_1 \, d\xi = 0.\tag{10}$$

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 NCONT = NBC + NINT - NDIM + 1 and is here equal to 2.

Note that in Eq. (5) we keep the term with the unfolding parameter ϵ that is explained in the tutorial SITDROP [1]. However, in the present tutorial one does not need to use it if the run is done with heterogeneous substrate or uses ρ as continuation parameter. However, if one wants to use the tutorial to look at drops on homogeneous substrate ($\rho = 0$) one might need it.

2 Runs:

The diagrams in Figs. 1-3 are determined through the continuation runs presented in the following table. The white fields describe what the individual runs do and mention important parameter settings including necessary changes. The grey fields give the `auto07` commands on the left when using the (modern) `Python` interface and on the right when using the more classic command line approach.

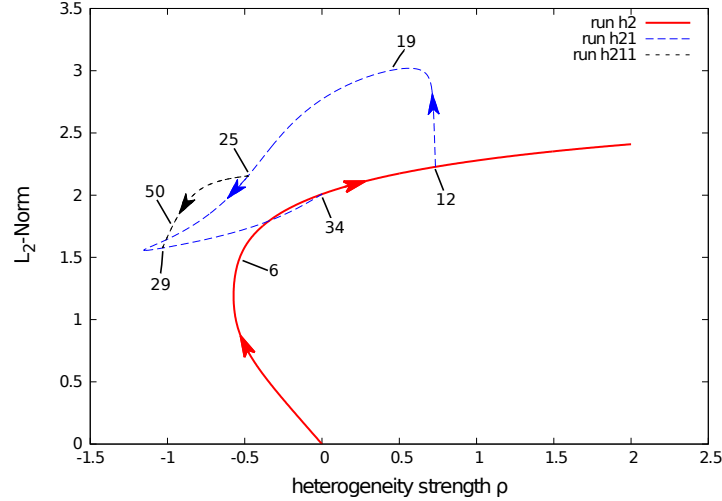


Figure 1: An illustration for runs 2, 21 and 211 (for respective linestyles see legend) of tutorial HETDROP is given. The L_2 -norm of steady solutions is shown in dependence of the principal continuation parameter heterogeneity strength ρ (par31)) for fixed domain size $L = 2P = 100$ (par(5)) and mean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

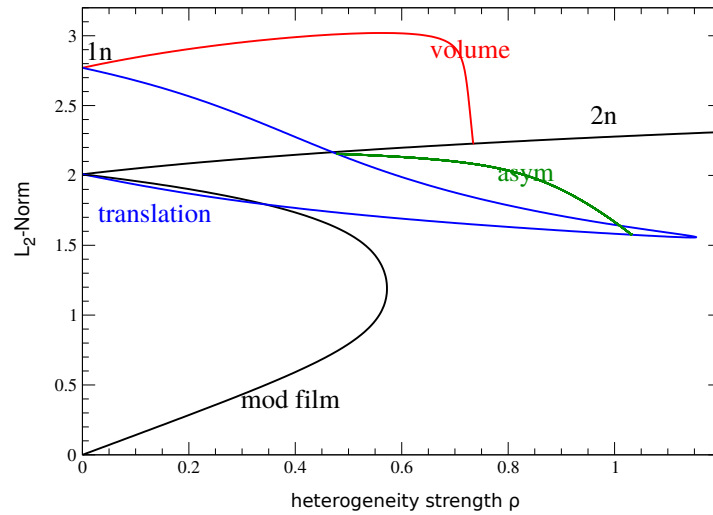


Figure 2: As equation (3) with (2) is invariant under the transformation $(\rho, x) \rightarrow (-\rho, x + P/2)$ and the used solution measures do not change under a shift in x , the bifurcation diagram in Fig. 1 is symmetric under $\rho \rightarrow -\rho$ and may therefore be completed by reflecting all curves at $\rho = 0$. The resulting complete bifurcation diagram in dependence of heterogeneity strength ρ (PAR(3)) is given here for $\rho \geq 0$. The various labels indicates how the branches are related.

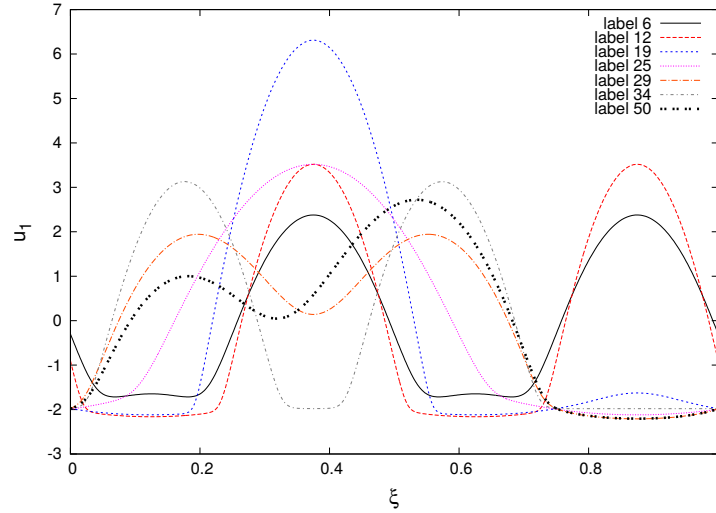


Figure 3: Steady film thickness profiles corresponding to Fig. (1) at heterogeneity strength ρ (PAR(3)) as given in the legend. The profiles are represented by $u_1(\xi) = h(\xi L) - h_0$ where $h_0 = 3$.

Python interface command line	Terminal command line
<i>auto</i>	
<p>run 1: Starting with a flat film on a homogeneous substrate ($\rho = 0$), determine steady solutions as a function of heterogeneity strength ρ. 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 ρ. Compute the branch of periodic solutions for $h_0 = 3$ continue in heterogeneity strength ρ (PAR(3)).</p> <p>Remaining true continuation parameters: C_1 (PAR(6)), E (PAR(9), we use NINT= 2)</p> <p>Parameters: IPS= 4, ISP= 2, ISW= 1, ICP= [3, 6, 9]</p> <p>Start data from function <i>stpnt</i> (IRS= 0) & check that ANZ= 1 in *.f90 file.</p> <p>Save output-files as b.h1, s.h1, d.h1.</p>	
<i>r1 = run(e = 'hetdrop', c = 'hetdrop.1', sv = 'h1')</i>	<i>@@R hetdrop 1</i> <i>@sv h1</i>
<p>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. Compute the branch of periodic solutions for $h_0 = 3$ continue in heterogeneity strength ρ (PAR(3)).</p> <p>Remaining true continuation parameters: C_1 (PAR(6)), E (PAR(9), we use NINT= 2)</p> <p>Parameters: IPS= 4, ISP= 2, ISW= 1, ICP= [3, 6, 9]</p> <p>Start data from function <i>stpnt</i> (IRS= 0) & check that ANZ= 2 in *.f90 file.</p> <p>Save output-files as b.h2, s.h2, d.h2.</p>	
<i>r2 = run(e = 'hetdrop', c = 'hetdrop.2', sv = 'h2')</i>	<i>@@R hetdrop 2</i> <i>@sv h2</i>

run 21: Restart at BP point of run 2; switch branch and follow side branch. It shows more BPs. Continue in heterogeneity strength ρ (PAR(3)), branch switching (ISW= -1), restart at LAB12 of run 2 (IRS= 12) Remaining true continuation parameters: C_1 (PAR(6)) Parameters: PS= 4, ISP= 2, ISW= -1, ICP= [3, 6, 9]. Save output-files as b.h21, s.h21, d.h21.	
<code>r21 = run(r2, e = 'hetdrop', c = 'hetdrop.21', sv = 'h21')</code>	<code>@@R hetdrop 21 h2 @sv h21</code>
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 ρ , look at the obtained profiles and understand the bifurcation structure. Continue in heterogeneity strength ρ (PAR(3)), branch switching (ISW= -1), restart at LAB25 of run 21 (IRS= 23) Remaining true continuation parameters: C_1 (PAR(6)) Parameters: IPS= 4, ISP= 2, ISW= -1, ICP= [3, 6, 9] Save output-files as b.h211, s.h211, d.h211.	
<code>r211 = run(r21, e = 'hetdrop', c = 'hetdrop.211', sv = 'h211')</code>	<code>@@R hetdrop 211 h21 @sv h211</code>
<code>clean()</code>	<code>@cl</code>

Table 1: Commands for running tutorial HETDROP.

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 tutorial. 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 $\rho \rightarrow -\rho$ and $h(x) \rightarrow h(x + P/2)$. 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 machines. 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.

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.

5 Outlook

Building on the here presented application of continuation techniques to thin-film equations to determine steady sitting drops on heterogeneous substrates you may advance to the tutorials HETDRIV [11] and ROTFFTW [12] investigating steady droplets on a heterogeneous inclined substrate and their stick-slip motion beyond depinning, respectively.

In the literature one also finds examples of the continuation of pinned ridge and drop states on inclined heterogeneous substrates in 2d [13] (also see Supplementary Material of [14]).

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