Münsteranian Torturials on Nonlinear Science

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Continuation

HETDRIV: steady drops on a heterogeneous substrate under lateral driving

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Abstract

The tutorial `HETDRIV` 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". The tutorial explores steady drops on a substrate with spatially varying wettability under the additional influence of lateral driving. You will calculate these steady states as a function of the main control parameters domain size, heterogeneity contrast and driving strength. The employed code package is `auto07p`. It is recommended to consider this tutorial after the tutorial `HETDROP` [1].

1 Model

The tutorial `HETDRIV` 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].
`HETDRIV` illustrates the calculation of pinned steady drop states that solve the dimensionless thin-film equation

$$\partial_t h \;=\; -\partial_x \left\{ Q(h)\,\partial_x \left[\underbrace{\partial_{xx} h - \partial_h f(h,x)}_{\text{pressure}} \right] + \chi(h) \right\} 6 \tag{1}$$

For an explanation of the basic structure of the equation see tutorial `SLIDROP` [7]. The important difference to the tutorial `SLIDROP` is that the Derjaguin pressure $-\partial_h f(h,x)$ now explicitly depends on the position x, i.e., we have a substrate with nonuniform wettability, i.e., the translational invariance is broken. Such a system was studied in [8, 9].
The technique introduced here was used in studies of droplets on heterogeneous inclined substrates [8, 9], and drops on the outside of rotating cylinders [10]. Related experiments and computer simulations are found in [11, 12].
Further, similar 1d codes were employed in [13] where also 2d results obtained with other continuation codes are presented.

For the case without lateral driving see tutorial `HETDROP` [1]. Here we assume a sinusoidal modulation of the long range contribution to the Derjaguin pressure:

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

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. Physically, the given form results in a modulation of equilibrium contact angle and adsorption layer (precursor film) thickness.
To study steady solutions, i.e., resting drops or modulated films, we set $\partial_t h = 0$ and integrate Eq. (1) once to obtain

$$0 \;=\; Q(h)\,\partial_x \left[\partial_{xx} h - \partial_h f(h,x)\right] + \chi(h) - C_0. \tag{3}$$

Here the constant C_0 stands for the mean flux that is constant for a steady solution. When writing Eq. (3) as a system of first-order ordinary differential equations on the interval [0, 1] (introducing $\xi = \frac{x}{L}$ $u_1 = h - h_0$, $u_2 = dh/dx$ and $u_3 = d^2h/dx^2$), and using $\chi(h) = \alpha Q(h)$, then one obtains the non-autonomous system (r.h.s depends explicitly on x)

$$\begin{aligned} \dot{u}_1 &= Lu_2 \\ \dot{u}_2 &= Lu_3 \\ \dot{u}_3 &= L\left[u_2 f_{u_1u_1}(u_1+h_0,x) + f_{u_1x}(u_1+h_0,x) - \alpha + \frac{C_0}{Q(u_1+h_0)}\right]. \end{aligned} \tag{4}$$

where L is the physical domain size, dots indicate derivatives with respect to ξ, and subscripts of f indicate partial derivatives. Such a non-autonomous system can not be handled by auto07p [5, 2, 14], therefore we transform it into an autonomous one. This is done by defining the position variable x to be another independent variable, i.e. $u_4 = x$ that as the other u_i depends on the independent variable ξ. One obtains the 4d dynamical system (NDIM = 4)

$$\begin{aligned} \dot{u}_1 &= L(u_2 - \epsilon f_{u_1}(u_1+h_0,u_4)) \\ \dot{u}_2 &= L(u_3 - \epsilon u_2) \\ \dot{u}_3 &= L\left[u_2 f_{u_1u_1}(u_1+h_0,u_4) + f_{u_1u_4}(u_1+h_0,u_4) - \alpha + \frac{C_0}{Q(u_1+h_0)}\right] \\ \dot{u}_4 &= L. \end{aligned} \tag{5}$$

Note that we have also introduced the unfolding parameter ϵ as in tutorial `SITDROP` [15], it is needed for the first runs that use a horizontal substrate. We use periodic boundary conditions for u_1, u_2 and u_3 that take the form

$$u_1(0) = u_1(1), \tag{6}$$
$$u_2(0) = u_2(1), \tag{7}$$
$$u_3(0) = u_3(1). \tag{8}$$

As 4th BC we 'pin' the physical position $u_4 = x$ to the computational position ξ by

$$u_4(0) = 0, \tag{9}$$

(i.e., NBC = 4). We also use an integral condition for mass conservation that takes the form

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

and four integral conditions that measure various energies (see f.90 file; these could be removed and the code would still work, they are normalised w.r.t. the flat film starting solution). In the very first run that starts from a state which is invariant with respect to translation we also employ an integral condition that breaks this invariance, (see tutorial `SITDROP` [15]).
As starting solution we use a slightly sinusoidally perturbed flat film of height h_0 at zero driving ($\alpha = 0$), fix the domain size to its critical value $L = L_c$ and set $u_4 = L\xi$. Here $L_c = 2\pi/k_c$ where $k_c = \sqrt{-f''(h_0)}$ is the critical wavenumber for the linear instability of a flat film of thickness h_0 on the homogeneous substrate (see tutorial `SITDROP` [15]). The starting value for C_0 is zero as well as $\epsilon = 0$.
The number of free (continuation) parameters is given by

$$\underbrace{\mathrm{NCONT}}_{\text{no. of continuation par.}} = \underbrace{\mathrm{NBC}}_{\text{boundary conditions}} + \underbrace{\mathrm{NINT}}_{\text{integral conditions}} - \underbrace{\mathrm{NDIM}}_{\text{dimensionality}} +1 \tag{11}$$

and is here equal to 7 or 6.

2 Runs:

The diagrams in Figs. 1-7 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.

Python interface command line	Terminal command line
auto	
run 1: Compute the branch of periodic solutions for $h_0 = 3$, continue in domain size. **Continuation parameters**: L (PAR(5)), C_0 (PAR(6)), ϵ (PAR(2)) and energies (PARs 36-38, 40), NINT= 6; **Settings**: IPS= 4, ISP= 2, ISW= 1, ICP= $[5, 6, 2, 40, 35, 36, 37]$, Start data from initial solution (IRS= 0) and check that ANZ= 1 in *.f90 file Save output-files as *b.h1, s.h1, d.h1.* Plot continuation results for analysis.	
r1 = run(e = 'hetdriv', c = 'hetdriv.1', sv = 'h1') *plot(r1)*	*@@R hetdriv 1* *@sv h1* *@pp h1*
run 11: Compute branch of periodic solutions for $h_0 = 3$, $L = 50$ and continue in heterogeneity strength (ρ positive), starting from previous solution h1. **Continuation parameters**: ρ (PAR(3)), C_0 (PAR(6)) , ϵ (PAR(2)) and energies (PARs 36-38, 40), NINT= 6; **Settings**: IPS= 4, ISP= 2, ISW= 1, ICP= $[3, 6, 2, 40, 35, 36, 37]$. Start data from LAB3 of run 1. Save output-files as `b.h11, s.h11, d.h11`. Plot continuation results for analysis.	
r11 = run(e = 'hetdriv', c = 'hetdriv.11', s = 'h1', sv = 'h11') *plot(r11)*	*@@R hetdriv 11 h1* *@sv h11* *@pp h11*
run 111: Compute periodic solutions for $h_0 = 3$, $L = 50$, $\rho = 0.75$, continue in lateral driving α. **Continuation parameters**: α (PAR(7)), C_0 (PAR(6)) and energies (PARs 36-38, 40), NINT= 5; **Settings**: IPS= 4, ISP= 2, ISW= 1, ICP= $[7, 6, 40, 35, 36, 37]$. start data from LAB18 of run 11. Save output-files as `b.h111, s.h111, d.h111` and plot results.	
r111 = run(e ='hetdriv',c = 'hetdriv.111',s = 'h11',sv = 'h111') *plot(r111)*	*@@R hetdriv 111 h11* *@sv h111* *@pp h111*
clean()	*@cl*

Table 1: Commands for running tutorial `HETDRIV`.

Run 1 Starting with a flat film on a homogeneous substrate ($\rho = 0$) without driving ($\alpha = 0$), determine steady solutions as a function of domain size L. Mean thickness $h_0 = 3$. We start at $L_c \approx 33$ and obtain profiles at domain sizes that are multiples of the heterogeneity period $P = 50$ (but heterogeneity remains switched off). (see fig.1,2.)

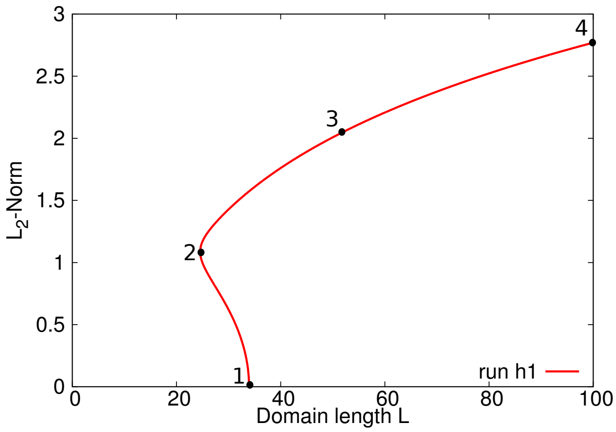

Figure 1: Graphic representation of the continuation of steady states with varying domain length L (PAR(5)). Shown is the Plot of the L2-norm vs domain length (**run h1**).

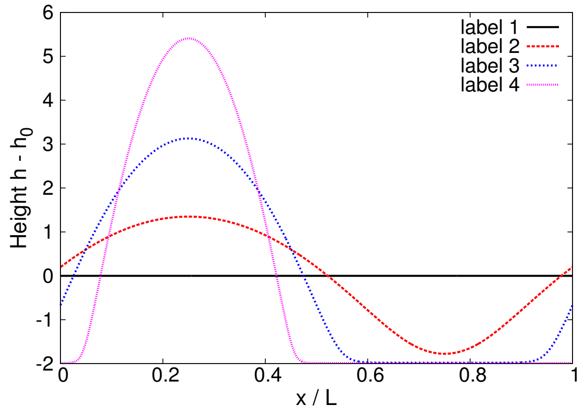

Figure 2: Shown are selected steady film profiles corresponding to the bifurcation curve in fig (1). (**run h1**).

Run 11 Starting with the drop solution at $L = 50$ on a homogeneous substrate ($\rho = 0$) without driving ($\alpha = 0$), determine steady solutions as a function of heterogeneity strength ρ (heterogeneity period $P = 50$). Mean thickness $h_0 = 3$ and domain size L is fixed.

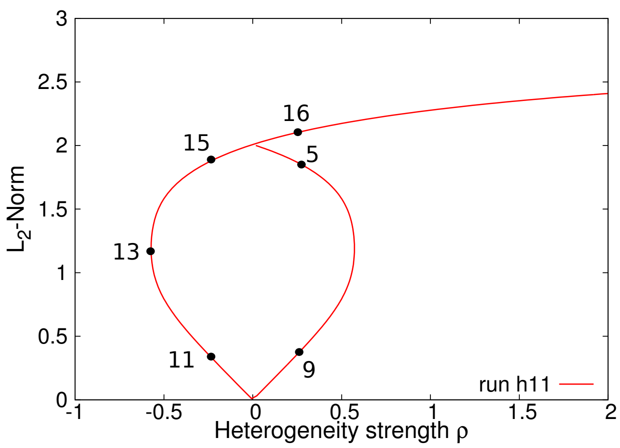

Figure 3: Plot of L_2-Norm vs. heterogeneity strength ρ.

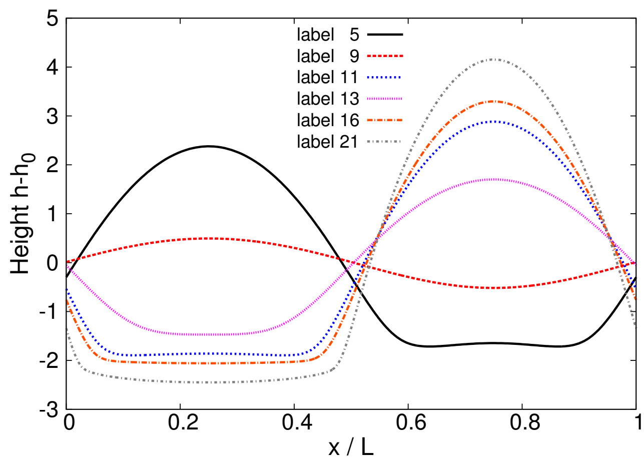

Figure 4: Selected Steady-state solutions corresponding to fig.(8).

Run 11b As run **11**, but going towards negative heterogeneity strength ρ. The following graphic shows the combination of run 11 and 11b.

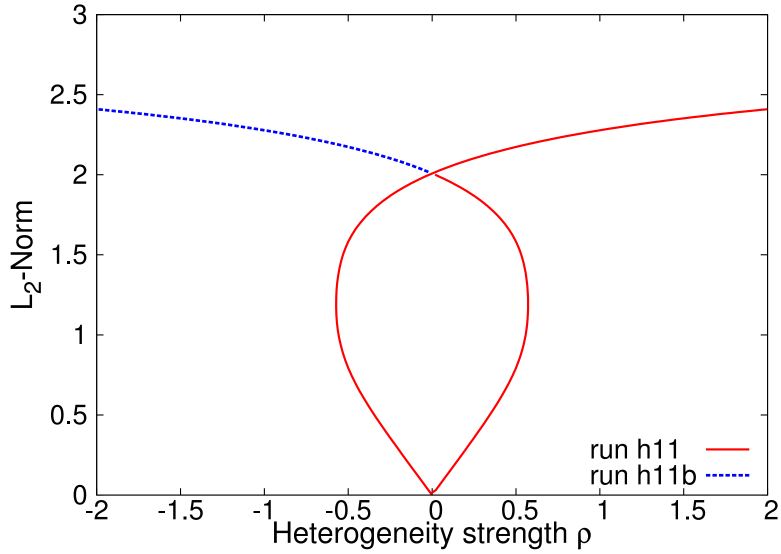

Figure 5: Combined results of run 11 and 11b.

Run 111 Starting with the drop solution at $L = 50$ on the heterogeneous substrate ($\rho = 0.75$) without driving ($\alpha = 0$), determine steady solutions as a function of lateral driving strength α ($P = L = 50$, $h_0 = 3$ and $\rho = 0.75$ fixed).

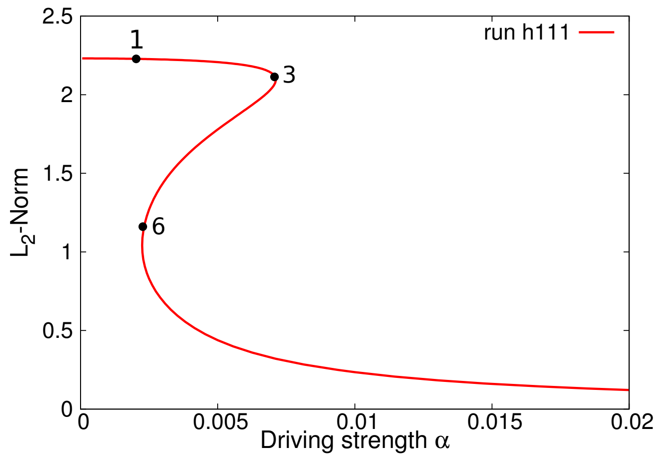

Figure 6: Graphical representation of L_2-Norm vs. driving strength α. A distinct film flattening can be observed for increased lateral driving strength (**run 111**).

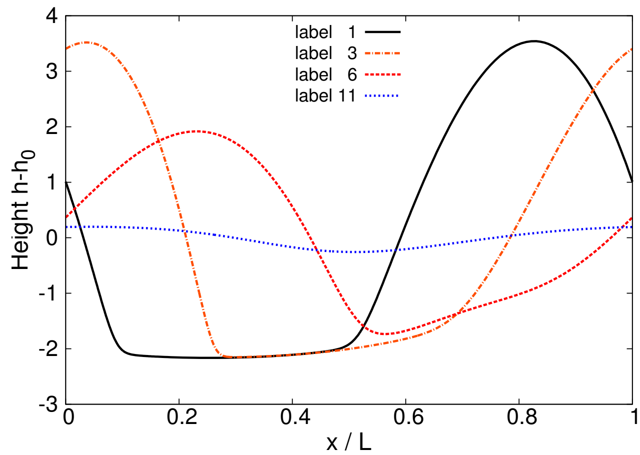

Figure 7: Selected profiles corresponding to the bifurcation curve of fig. (6)(**run 111**).

3 Remarks:

- Screen output and command line commands are also provided in README file, more info on continuation parameter in table. All runs also measure 4 energies.
- run 1 is in principle identical to run 1 in the tutorial `SITDROP` [15] but is here performed within a more complicated system of equations, which also describes heterogeneity and driving.
- The hetdriv.f90 file provides another 4 integral conditions that are used in all runs of the tutorial. They allow for a determination of the total energy of the obtained steady state solutions(PAR(40)), as well as of its components (surface energy(PAR(35)), wetting energy(PAR(36)) and potential energy(PAR(37))).
- The constant C_0 corresponds to the flow. (you may, for example, plot C_0 against the measured Energies with *@pp h111*)

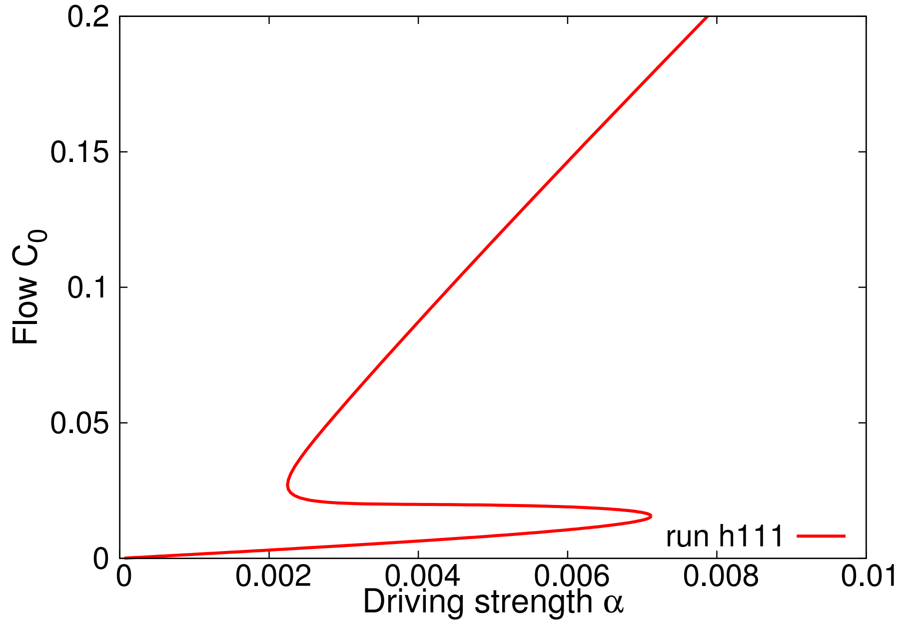

Figure 8: Plot of surface flow (C_0) vs. lateral driving parameter α.

4 Tasks:

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

- Redo the runs for other values of h_0. What do you observe? (compare fig. 9)
- Deactivate the integral conditions that measures the energy of the solutions. (within subroutine ICND in .f90 file)
- Modulate the entire Derjaguin pressure instead of the long-range part (see eq.(1)). This corresponds to a modulation of the contact angle at fixed precursor film height.
- Replace the used Derjaguin pressure by a different one that you get from the literature (See tasks of tutorial `SITDROP` [15]).
- Look at two periods of the heterogeneity and get a full picture that shows what happens with all the solutions found in tutorial `HETDROP` [1] under lateral driving (you may have to vary the period length, -number and the domain size in the .f90 file.)

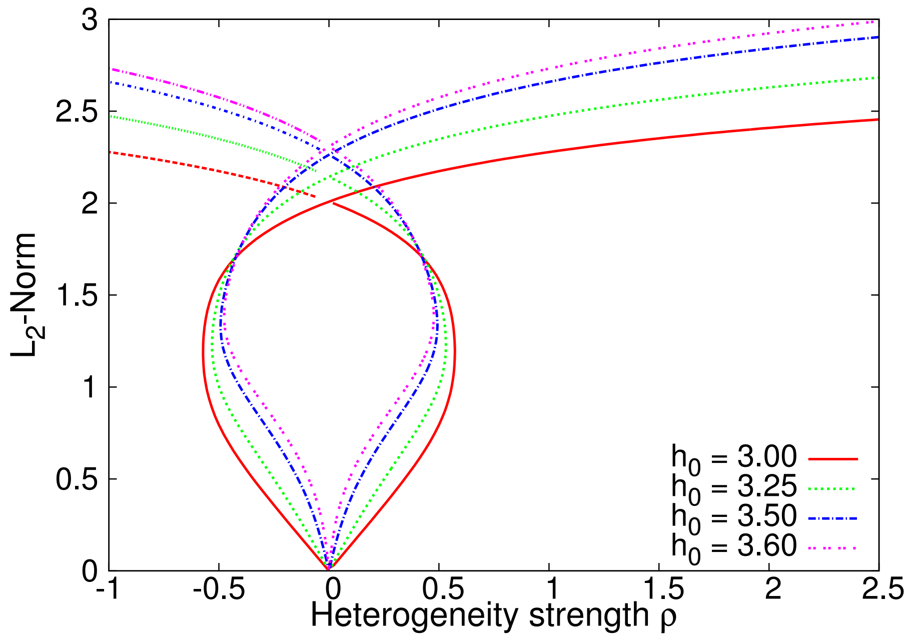

Figure 9: Plot of heterogeneity parameter ρ vs. L_2-Norm of steady state solution with different average film thicknesses H (h_0: 3.0 (red), 3.25 (blue), 3.5 (green), 3.75 (pink)).

References

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