

Münsteranian Torturials on Nonlinear Science

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Continuation

LINDROP: linear stability of steady states on a horizontal homogeneous substrate

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Abstract

The tutorial LINDROP 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 calculates the same 1d steady states as the tutorial SITDROP [1], and additionally determines their linear stability (in 1d and 2d) with respect to time-dependent perturbations. You will calculate the dispersion relation (growth rate over transversal wave number of the Plateau-Rayleigh instability of liquid ridges). Steady states and their stability are continued in various parameters. The employed code package is `auto07p`. It is recommended to consider this tutorial after the tutorial SITDROP [1].

1 Model

The tutorial LINDROP 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].

LINDROP illustrates the calculation of steady drop and hole states of the dimensionless thin-film equation in 1D *together* with their linear stability w.r.t. 1D and 2D modes. This is possible within `auto07p` [5, 2, 7], as real eigenvalues can be detected as branching points (cf. `auto07p` demo `lin` [5, 2, 7]).

As the evolution equation is a gradient dynamics (of a similar form as the Cahn-Hilliard equation studied in the tutorial ACCH [8]), one knows that all eigenvalues are real (see, e.g., [9]). In Ref. [10] the technique is used for films and ridges on homogeneous and heterogeneous substrates.²

The thin film evolution equation is

$$\partial_t h = \nabla \cdot \left\{ Q(h) \nabla \frac{\delta F}{\delta h} \right\} \quad \text{with} \quad F[h] = \int_A dr \left[\frac{\gamma}{2} (\nabla h)^2 + f(h) \right], \quad (1)$$

where $Q(h) = h^3/3\eta$ is the mobility factor, γ is the surface tension, and η is the dynamic viscosity. Performing the variaton, the equation becomes (now nondimensionalised)

$$\partial_t h = -\nabla \cdot \{ Q(h) \nabla [\Delta h - \partial_h f(h)] \} \quad (2)$$

For further explanations see tutorials SITDROP [1] where a 1d version of Eq. (1) is used, and ACCH [8] where a 1d version of the closely related Cahn-Hilliard equation is used.

To determine steady states in 1d and their linear stability in 1d and 2d one needs to continue steady states $h_0(x)$, i.e. solutions of³

$$0 = \partial_{xx} h_0(x) - \partial_h f(h_0) + C_1. \quad (3)$$

²A related strategy for cases where eigenvalues are complex needs starting values for eigenvalues and eigenfunctions obtained through a different technique [11, 12].

³Remember, the constant C_1 accounts for external conditions like chemical potential, vapor pressure or mass conservation. Here we consider the latter case where C_1 takes the role of a Lagrange multiplier for mass conservation.

together with solutions of the eigenvalue problem obtained when Eq. (2) is linearized about $h_0(x)$. We use the ansatz $h(x, y, t) = h_0(x) + \varepsilon h_1(x) \exp(\beta t + i q y)$, i.e., we assume that the steady 1d drops are actually ridges in 2d. They might be unstable with respect to 1d modes ($q = 0$) or/and with respect to 2d modes where the modulation in the transversal direction (y -direction, along the ridge) is harmonic. Introducing the ansatz into Eq. (2) and linearizing in $\varepsilon \ll 1$, gives the linear eigenvalue problem

$$\beta h_1(x) = \mathcal{L}[h_0, q] h_1(x) \quad (4)$$

where the growth rate β is the eigenvalue, $h_1(x)$ is the eigenvector (or -mode) and $\mathcal{L}[h_0, q]$ is a fourth order linear operator acting on $h_1(x)$. It depends nonlinearly on h_0 , $\partial_x^i h_0$, the transversal wavenumber q and all the other parameters of the problem. In expanded form the equation is

$$\begin{aligned} \beta h_1 &= -\nabla \cdot \{ \partial_h Q_0 h_1 \overbrace{\nabla [\Delta h_0 - \partial_h f_0]}^{=0} \} - \nabla \cdot \{ Q_0 \nabla [\Delta h_1 - (\partial_{hh} f_0) h_1] \} \\ &= -\nabla \cdot \{ Q_0 \nabla [\Delta h_1 - (\partial_{hh} f_0) h_1] \} \\ &= -\partial_x \{ Q_0 \partial_x [(\partial_{xx} - q^2) h_1 - (\partial_{hh} f_0) h_1] \} + Q_0 q^2 [(\partial_{xx} - q^2) h_1 - (\partial_{hh} f_0) h_1] \\ &= -Q_0 \partial_{xx} [(\partial_{xx} - q^2) h_1 - (\partial_{hh} f_0) h_1] - (\partial_x Q_0) \partial_x [(\partial_{xx} - q^2) h_1 - (\partial_{hh} f_0) h_1] \\ &\quad + Q_0 q^2 [(\partial_{xx} - q^2) h_1 - (\partial_{hh} f_0) h_1] \end{aligned} \quad (5)$$

where we used Eq. (3) to eliminate the first term in the first line of Eq. (5). Here, an subscript 0 indicates that the corresponding function has to be taken at h_0 . With this we have a second order equation for h_0 (Eq. (3)) that we have to solve together with the 4th order equation for h_1 (Eq. (5)). To use `auto07p` [5, 2, 7], we first write the two equations as a system of six first-order autonomous ordinary differential equations on the interval $[0, 1]$. Therefore, we introduce the variables $u_1 = h_0 - \bar{h}$ and $u_2 = dh_0/dx$, and obtain from Eq. (3) the first two equations

$$\begin{aligned} \dot{u}_1 &= L u_2 - \alpha [f'(\bar{h} + u_1) - C_1] \\ \dot{u}_2 &= L [f'(\bar{h} + u_1) - C_1]. \end{aligned} \quad (6)$$

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 $u_1(\xi)$ and $u_2(\xi)$ correspond to the correctly scaled physical fields $h(L\xi)$ and $\partial_x h(L\xi)$. We employ the 'unfolding parameter' α that transforms the conservative in a 'virtual' dissipative system (with the same solutions) as explained in tutorials SITDROP [1] and ACCH [8].

Further we introduce $u_3 = h_1$, $u_4 = dh_1/dx$, $u_5 = d^2 h_1/dx^2$ and $u_6 = d^3 h_1/dx^3$ and write Eq. (5) as

$$\begin{aligned} \dot{u}_3 &= L u_4 \\ \dot{u}_4 &= L u_5 \\ \dot{u}_5 &= L u_6 \\ \dot{u}_6 &= L \left\{ -\frac{\beta u_3}{Q_0} + q^2 u_5 + \partial_{xx} (h_1 \partial_{hh} f_0) - \frac{\partial_x Q_0}{Q_0} [(u_6 - q^2 u_4 - \partial_x (h_1 \partial_{hh} f_0))] \right. \\ &\quad \left. + q^2 [u_5 - q^2 u_3 - f''(\bar{h} + u_1) u_3] \right\} \end{aligned} \quad (7)$$

where

$$\begin{aligned} \partial_x (h_1 \partial_{hh} f_0) &= f'''(\bar{h} + u_1) u_2 u_3 + f''(\bar{h} + u_1) u_4 \\ \partial_{xx} (h_1 \partial_{hh} f_0) &= f''''(\bar{h} + u_1) u_2^2 u_3 + f'''(\bar{h} + u_1) (\partial_{xx} h_0) u_3 + 2f'''(\bar{h} + u_1) u_2 u_4 + f''(\bar{h} + u_1) u_5 \end{aligned} \quad (8)$$

and $\partial_{xx}h_0 = f'(\bar{h} + u_1) - C_1$ [Eq. (3)]. This means, in total we have $\text{NDIM} = 6$. We use periodic boundary conditions for all u_i ($\text{NBC} = 6$) that take the form

$$u_i(0) = u_i(1) \quad (9)$$

and integral conditions for mass conservation of h_0 and computational pinning (to break the translational symmetry that the solutions h_0 have on the considered homogeneous substrate) ($\text{NINT} = 2$). The integral condition for mass conservation takes the form

$$\int_0^1 u_1 d\xi = 0. \quad (10)$$

Note that mass conservation for the perturbation is automatically fulfilled as the linearised thin film equation still describes a conserved dynamics. To also account for evaporative dynamics a non-conserved term would need to be added to Eq. (2) [9].

As starting solution for h_0 we use a 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 . This results in $C_1 = f'(h_0)$ as starting value for C_1 . The starting solution for h_1 is the trivial eigenfunction $h_1 = 0$. We also set $\beta = 0$ and fix q at some value.

The number of free (continuation) parameters is given by $\text{NCONT} = \text{NBC} + \text{NINT} - \text{NDIM} + 1$ and is here equal to 3.

2 Runs:

The diagrams in Figs. 1 and 2 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 `auto07p` commands on the left when using the (modern) `Python` interface and on the right when using the more classic command line approach.

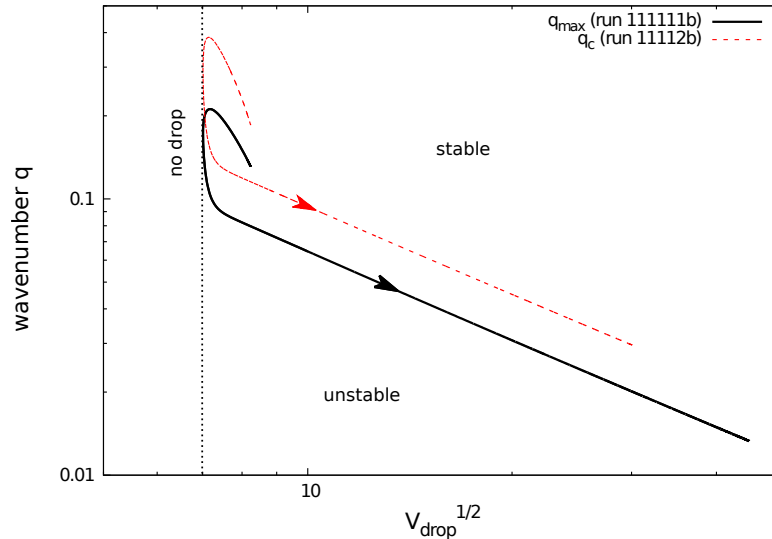


Figure 1: Stability diagram showing the critical transversal wavenumber q_c (PAR(8)) and the fastest growing transversal wavenumber q_{\max} (PAR(8)) as a function of the square root of the drop volume, that is related to the continuation parameter domain size by $V = L(\bar{h} - 1)$ (L is PAR(5)). Shown are results for the subcritical and supercritical part of the branch of steady hole and drop solutions of Eq. (1). The mean film height is $\bar{h} = 3.0$. The results are obtained in runs 111111 (q_{\max}) and 11112 (q_c) described in Table 4.1.

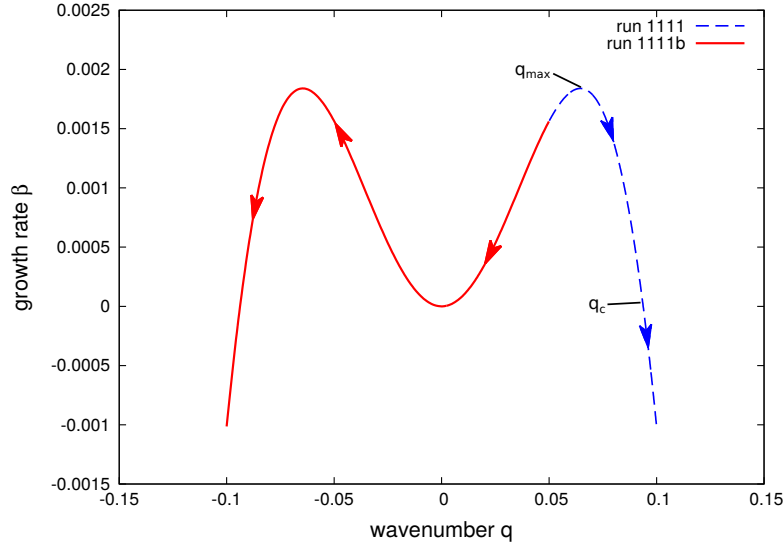


Figure 2: Dispersion-relation of standard and 'b' runs. The wavenumber q corresponds to (PAR(8)) and the growth rate β corresponds to (PAR(7)). The two wavenumbers used in Fig. 1 are marked as q_{max} and q_c .

Python interface command line	Terminal command line
<i>auto</i>	
<p>run 1: Determine steady solutions as a function of domain size L up to $L = 100.$, starting at the critical L_c with one period of a small-amplitude sinusoidal solution. Mean thickness $h_0 = 3$ is fixed. One finds that the primary bifurcation is subcritical, and that the branch turns towards larger L at a saddle-node bifurcation at some $L_{sn} < L_c$. Transversal wavenumber fixed at some value $q \neq 0$.</p> <p>Continuation parameters: L (PAR(5)), C_1 (PAR(6)) and α (PAR(2));</p> <p>Other output parameters: none</p> <p>Settings: IPS= 4, ISP= 0, ISW= 1, NINT= 2, ICP= [5, 6, 2]</p> <p>Start data: from function <i>stpnt</i> (IRS= 0)</p>	
<code>r1 = run(e = 'lindrop', c = 'lindrop.1', sv = 'ld1')</code>	<code>@@R lindrop 1 @sv ld1</code>
<p>run 11: Restart at domain size $L = 100$, change eigenvalue β from zero. Eigenvalues are detected as branching points.</p> <p>Continuation parameters: β (PAR(7)), C_1 (PAR(6)) and α (PAR(2));</p> <p>Other output parameters: none</p> <p>Settings: IPS= 4, ISP= 2, ISW= 1, NINT= 2, ICP= [7, 6, 2]</p> <p>Start data: LAB5 of run 1: IRS= 5</p> <p>save output-files as <code>b.ld11</code>, <code>s.ld11</code>, <code>d.ld11</code></p>	
<code>r11 = run(r1, e = 'lindrop', c = 'lindrop.11', sv = 'ld11')</code>	<code>@@R lindrop 11 ld1 @sv ld11</code>

<p>run 111: Restarting at a branching point, we switch branch. This 'blows up' the correct eigenfunction h_1 from zero. We measure the norm (by switching on the third integral condition through $NINT = 3$) and stop when it reaches one.</p> <p>Continuation parameters: β (PAR(7)), C_1 (PAR(6)), α (PAR(2)) and norm (PAR(9));</p> <p>Other output parameters: none</p> <p>Settings: IPS= 4, ISP= 2, ISW= -1, NINT= 3, ICP= [7, 6, 2, 9]</p> <p>Start data: LAB9 of run 11: IRS= 9</p> <p>save output-files as b.ld111, s.ld111, d.ld111</p>	
<i>r111 = run(r11, e = 'lindrop', c = 'lindrop.111', sv = 'ld111')</i>	<i>@@R lindrop 111 ld11 @sv ld111</i>
<p>run 1111: Now we are free to continue in q and β to get the transversal dispersion relation for any solution. Norm, L remain fixed.</p> <p>Continuation parameters: β (PAR(7)), q (PAR(8)), C_1 (PAR(6)) and α (PAR(2));</p> <p>Other output parameters: none</p> <p>Settings: IPS= 4, ISP= 2, ISW= 1, NINT= 3, ICP= [7, 8, 6, 2]</p> <p>Start data: LAB15 of run 111: IRS= 15</p> <p>save output-files as b.ld1111, s.ld1111, d.ld1111</p>	
<i>r1111 = run(r111, e = 'lindrop', c = 'lindrop.1111', sv = 'ld1111')</i>	<i>@@R lindrop 1111 ld111 @sv ld1111</i>
<p>run 11111 and 111111: Continue maximum of dispersion relation as fold using domain size as additional continuation parameter. Starting run 11111 and proper continuation run 111111.</p> <p>Continuation parameters: β (PAR(7)), q (PAR(8)), C_1 (PAR(6)), α (PAR(2)), L (PAR(5));</p> <p>Other output parameters: none</p> <p>Settings: IPS= 4, ISP= 2, ISW= 2, NINT= 3, ICP= [7, 8, 6, 2, 5]; in run 111111 we set ILP= 0 and ISP= 0 to avoid spurious LP and BR detection, respectively.</p> <p>Start data: run 11111: LAB16 of run 1111: IRS= 16 and run 111111: LAB19 of run 11111: IRS= 19</p> <p>save output-files</p>	
<i>r11111 = run(r1111, e = 'lindrop', c = 'lindrop.11111', sv = 'ls11111')</i>	<i>@@R lindrop 11111 ld1111 @sv ld11111</i>
<i>r111111 = run(r11111, e = 'lindrop', c = 'lindrop.111111', sv = 'ls111111')</i>	<i>@@R lindrop 111111 ld11111 @sv ld111111</i>
<p>run 11112: Continue zero-crossing of dispersion relation, using also domain size as continuation parameter.</p> <p>Continuation parameters: q (PAR(8)), C_1 (PAR(6)), α (PAR(2)), L (PAR(5));</p> <p>Other output parameters: none</p> <p>Settings: IPS= 4, ILP= 0, ISP= 0, ISW= 1, NINT= 3, ICP= [8, 6, 2, 5];</p> <p>Start data: LAB17 of run 1111: IRS= 17</p> <p>save output-files</p>	
<i>r11112 = run(r1111, e = 'lindrop', c = 'lindrop.11112', sv = 'ls11112')</i>	<i>@@R lindrop 11112 ld1111 @sv ld11112</i>
<i>clean()</i>	<i>@cl</i>

Table 1: Commands for running demo LINDROP.

3 Remarks:

- Runs with a **b** at the end (see README_lindrop) correspond to the previous one, but going into the opposite direction.
- This procedure can be repeated for other eigenvalues to get a more complete picture (E.g. try for a pair of drops by repeating everything setting number of periods to $NN = 2$ in the f90 file.)
- Screen output and command line commands are provided in file README_lindrop.
- In thermodynamic context, the constant C_1 corresponds to the negative of the chemical potential.
- 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.
- 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.,

- redo sequence of runs for other values of h_0 , e.g., 1.27, 1.5, 2.5, 5.0, 10.0.
- Investigate several eigenvalues. Look at eigenfunctions. Are there eigenvalues that are positive at $q = 0$ or cross zero for fixed $q = 0$ when changing other parameters?
- Try to run a continuation with fixed C_1 (you need to 'set free' another parameter). Do your stability results change?

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