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Continuation

CCH: Travelling drops and waves in the convective Cahn-Hilliard equation

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8 cch: Travelling drops and waves in the convective Cahn-Hilliard equation

The tutorial CCH explores the convective Cahn-Hilliard equation. Compared to the Cahn-Hilliard equation, it features an added driving force. You will calculate stationary solutions representing moving density 'drops' and continue them using the driving force as control parameter.

8.1 Model

This demo illustrates the calculation of travelling drop and wave solutions of the convective Cahn-Hilliard equation

$$\partial_t \phi \;=\; M\partial_{xx}\frac{\delta F}{\delta \phi} - D\phi\partial_x\phi \;=\; -M\partial_{xx}\left[\kappa\partial_{xx}\phi - \partial_\phi f(\phi)\right] - D\phi\partial_x\phi \tag{8.1}$$

where M is a constant mobility factor, $\phi(x,t)$ is the independent (field) variable (depending on context it might represent a density ρ or a concentration c), and D is the strength of a lateral driving (electric field, gravity, etc.). The sign is chosen such that $D > 0$ corresponds to a force acting towards the right (towards larger x). The term in square brackets corresponds to a (non-equilibrium) chemical potential. The one used here is the same as in the tutorial `acch` [1] where it is explained in detail. We use the free energy functional

$$F[\phi] \;=\; \int_L dx\left[\frac{\kappa}{2}(\partial_x\phi)^2 + f(\phi)\right], \tag{8.2}$$

where L is the domain size. The term in square brackets consists of a 'curvature' contribution $\partial_{xx}\phi$ and a local contribution $\partial_\phi f(\phi)$ written as the derivative of a local free energy $f(\phi)$. The latter has a particular form for each studied problem. In the tutorial we use a simple double well potential (as in the tutorial `acch` [1]).

$$f(\phi) = \frac{a}{2}\phi^2 + \frac{b}{4}\phi^4 \tag{8.3}$$

For background information on the non-convective ($D = 0$) Cahn Hilliard see [2], for the convective equation see Refs. [3, 4]. The equation may be seen as an approximation of the equation describing a sliding drop on an incline (see [5]).

The present aim is to study travelling drops and waves that are steady in some co-moving frame, i.e., the drops or waves move with constant speed v and constant shape. We introduce the coordinate in the frame moving with v by $\tilde{x} = x - vt$ and obtain from Eq. (8.1) after dropping the tildes

$$-\,v\partial_x\,\phi \;=\; -M\partial_{xx}\left[\kappa\partial_{xx}\phi - \partial_\phi f(\phi)\right] - D\phi\partial_x\phi \tag{8.4}$$

Eq. (8.4) is integrated once to obtain

$$0 \;=\; -M\partial_x\left[\kappa\partial_{xx}\phi - \partial_\phi f(\phi)\right] - \frac{D}{2}\phi^2 + v\phi + C_0 \tag{8.5}$$

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

To use the continuation toolbox `auto07p` [6], we first write the 3rd order ordinary differential equation (ODE) (8.5) as a system of first-order ODEs on the interval $[0,\ 1]$. Therefore, we introduce the variables $u_1 = \phi - \phi_0$, $u_2 = d\phi/dx$ and $u_2 = d^2\phi/dx^2$, and obtain from equation (8.5) the 3d dynamical system ($\mathrm{NDIM} = 3$)

$$\begin{aligned} \dot{u}_1 &= Lu_2 \\ \dot{u}_2 &= Lu_3 \\ \dot{u}_3 &= \tfrac{L}{\kappa}\left[u_2 f''(u_1 + h_0) + \tfrac{1}{M}\left[-\tfrac{D}{2}\phi^2 + v(u_1+\phi_0) + C_0\right]\right]. \end{aligned} \tag{8.6}$$

where L is the physical domain size, and dots and primes denote derivatives with respect to $\xi \equiv x/L$ and ϕ, 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 $\phi(L\xi) - \phi_0$, $\partial_x\phi(L\xi)$ and $\partial_{xx}\phi(L\xi)$. We use periodic boundary conditions for all u_i ($\mathrm{NBC} = 3$) that take the form

$$u_1(0) = u_1(1), \tag{8.7}$$

$$u_2(0) = u_2(1), \tag{8.8}$$

$$u_3(0) = u_3(1), \tag{8.9}$$

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

$$\int_0^1 u_1 \,\mathrm{d}\xi = 0. \tag{8.10}$$

There are two ways to start the continuation. Either (i) one sets $D = 0$ and uses as in the tutorial `ACCH` the starting solution consisting of small amplitude harmonic modulation of wavelength $L_c = 2\pi/k_c$ where $k_c = \sqrt{-f''(\phi_0)}$ is the critical wavenumber for the linear instability of a homogeneous state $\phi(x) = \phi_0$ and also sets the starting values $v = 0$ and $C_0 = 0$; or (ii) one starts at some $D \neq 0$, uses a small amplitude harmonic starting solution with $L_c = 2\pi/k_c$ and initialises $v = D\phi_0$ and $C_0 = -v\phi_0 + D\phi_0^2/2$. In the tutorial we use option (i).

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

8.2 Runs:

Python interface command line	Terminal command line
auto	
run 1: Determine steady solutions on the horizontal substrate ($D = 0$)as a function of domain size L, starting at the critical L_c with a small amplitude sinusoidal solution. Mean value of ϕ is fixed. Compute the branch of periodic solutions for $\phi_0 = 0$ continued in L (PAR(5)) up to $L = 500$. **Remaining true continuation parameters:** C_0 (PAR(6)) and v (PAR(7)) **Parameter:** IPS= 4, ISP= 0, ISW= 1, ICP= $[5, 6, 7]$, Start data from function *stpnt* (IRS= 0) Save output-files as `b.tt1, s.tt1, d.tt1`	
r1 = run(e = 'cch', c = 'cch.1', sv = 'tt1')	*@@R cch 1* *@sv tt1*
run 11: Restart at domain size $L = 50$, keep value ϕ_0 fixed and increase driving strength D from zero to observe transition from moving drops to waves. Continue in driving D (PAR(4)) for fixed domain size $L = 50$. Stop at $D = 10$. **Remaining true continuation parameters:** C_0 (PAR(6)) and and v (PAR(7)) **Other output:** absolute value of minimal and maximal slope of ϕ (PAR(47) and PAR(48)) **Parameters:** IPS= 4, ISP= 0, ISW= 1, ICP= $[4, 6, 7, 47, 48]$, Start at LAB4 of run 1: IRS= 4 Save output-files as `b.tt11, s.tt11, d.tt11`	
r11 = run('tt1', e = 'cch', c = 'cch.11', sv = 'tt11')	*@@R cch 11 tt1* *@sv tt11*
clean()	*@cl*

Table 8.1: Commands for running demo `CCH`.

8.3 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 tutorial `acch` [1] one may define other integral condition to determine integral measures one might be interested in.
- Screen output and command line commands are provided in README file.

8.4 Tasks:

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

2, 21 Redo runs 1 and 11 for other values of ϕ_0.

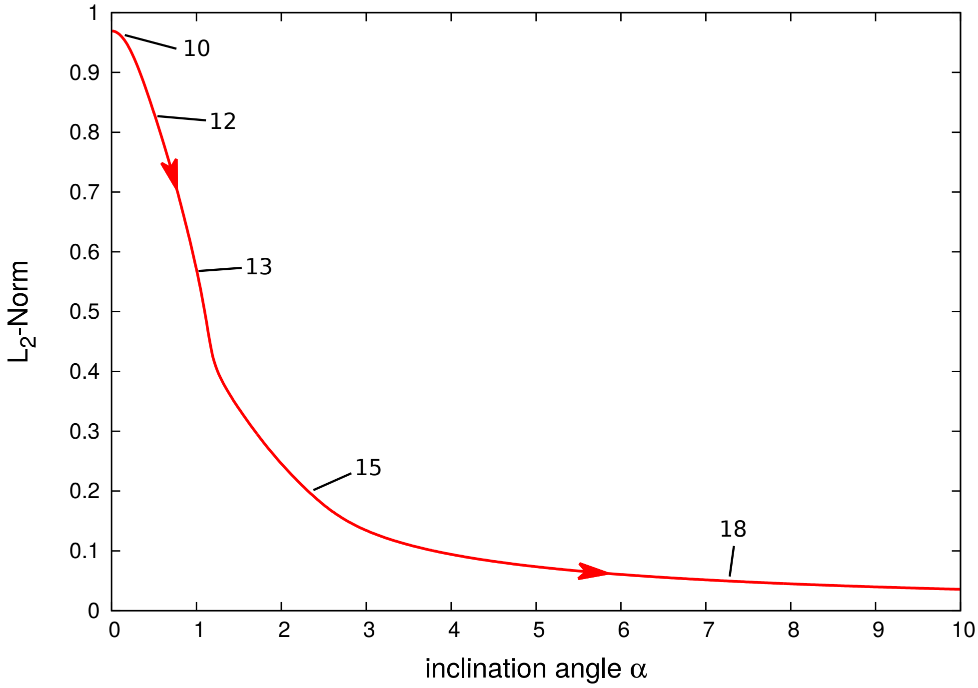

Figure 8.1: Continuation of inlcination angle α (par(4)).

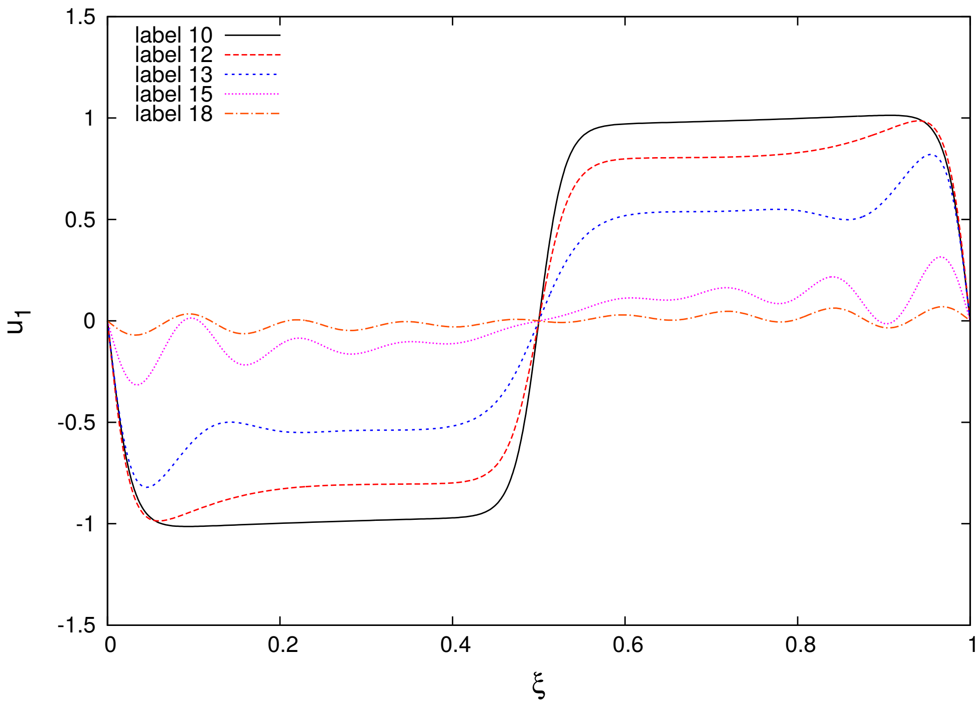

Figure 8.2: Solutions $u_1(\xi)$ i.e. $\phi(\xi L) - \phi_0$ corresponding to Fig. (8.1).

111 Restart at solutions obtained in run 11, continue again in D but now keep the flux C_0 fixed. You need to 'set free' another parameter, eg. ϕ_0.

112 Think about a way how you could do as in run 111, but keeping the flux in the laboratory frame fixed.

12 As run 11, but restart at other solutions obtained in run 1, eg. at $L = 100, 200, 300, \ldots$

- Include additional integral condition(s), to measure characteristics of interest. These might be the surface energy, or wetting energy, or the total energy dissipation.
- Replace the used driving $(D/2)\partial_x(\phi^2)$ by $(D/n)\partial_x(\phi^n)$ with other powers n. Do you observe changes in the symmetries of solutions and solution families?

References

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

[2] J. S. Langer. "An introduction to the kinetics of first-order phase transitions". In: *Solids far from Equilibrium*. Ed. by C. Godreche. Cambridge University Press, 1992. Chap. 3, pp. 297–363.

[3] A. A. Golovin et al. "Convective Cahn-Hilliard models: From coarsening to roughening". In: *Phys. Rev. Lett.* 86 (2001), pp. 1550–1553. DOI: 10.1103/PhysRevLett.86.1550.

[4] MA Zaks et al. "Periodic stationary patterns governed by a convective Cahn-Hilliard equation". In: *SIAM J. Appl. Math.* 66 (2006), pp. 700–720. DOI: 10.1137/040615766.

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[6] 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.