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# Continuation

## ACCH: Steady states of Allen-Cahn and Cahn-Hilliard equation

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# 5 acch: Steady states of Allen-Cahn and Cahn-Hilliard equation

The tutorial ACCH explores steady states of the Allen-Cahn and the Cahn-Hilliard equation with periodic boundary conditions. These equations describe, e.g., the dynamics of concentration profiles of binary fluids or the dynamics of magnetization. You will calculate steady solutions and continue them using domain size and mean concentration as control parameters.

## 5.1 Model

This demo illustrates the calculation of spatially varying steady solutions of the Allen-Cahn equation (non-conserved dynamics)

$$\partial_t \phi \;=\; -D\left[\frac{\delta F}{\delta \phi} - \mu\right] \;=\; D\left[\kappa \partial_{xx}\phi - \partial_\phi f(\phi) + \mu\right] \tag{5.1}$$

and the Cahn-Hilliard equation (conserved dynamics)

$$\partial_t \phi \;=\; M\partial_{xx}\frac{\delta F}{\delta \phi} \;=\; -M\partial_{xx}\left[\kappa \partial_{xx}\phi - \partial_\phi f(\phi)\right] \tag{5.2}$$

where $D$ and $M$ are respective constant mobility factors (not relevant for steady states), $\phi(x,t)$ is the independent (field) variable (depending on context it might represent a density $\rho$, a magnetisation $m$ or a concentration $c$), $\mu$ is a parameter that may stand for an external field, chemical potential or Lagrange multiplier (see below). In both cases we use the free energy functional

$$F[\phi] \;=\; \int_L dx\left[\frac{\kappa}{2}(\partial_x\phi)^2 + f(\phi)\right], \tag{5.3}$$

where $L$ is the domain size. For background information see [1]. The term in square brackets represents a (in general) non-uniform chemical potential and 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 demo we use a simple double well potential

$$f(\phi) = \frac{a}{2}\phi^2 + \frac{b}{4}\phi^4 \tag{5.4}$$

that may be seen as a Taylor expansion of the 'true' potential about the critical point related to the $1^{st}$ order phase transition. The parameter $b > 0$ and $a$ is arbitrary. The critical point is at $a = a_c = 0$.

To study steady solutions, i.e., resting non-uniform or uniform profiles, we set $\partial_t\phi = 0$ and obtain from the Allan-Cahn Eq. (5.1) the expression

$$0 \;=\; \kappa\partial_{xx}\phi - \partial_\phi f(\phi) + \mu. \tag{5.5}$$

In the case of the Cahn-Hilliard Eq. (5.2) one has to integrate Eq. (5.2) twice (this is possible as the first integration constant is zero for systems without through-flow). Remarkably, we obtain again Eq. (5.5) where $\mu$ is now introduced as an integration constant.

As mentioned above, in the context of the Allan-Cahn equation the constant $\mu$ accounts for external conditions like chemical potential, vapor pressure or an external magnetic field in a straightforward way. However, in the context of the Cahn-Hilliard equation that represents a conserved dynamics one might want to consider steady solutions of a fixed mean concentration $\bar{\phi} = \int_L \phi(x)dx$. Then $\mu$ takes the role of a Lagrange multiplier for the conservation of $\phi$.

To use the continuation toolbox `auto07p` [2]), we first write (5.5) as a system of first-order autonomous ordinary differential equations on the interval $[0,\ 1]$. To do so, we introduce the variables $u_1 = \phi$ and $u_2 = d\phi/dx$, and obtain from equation (5.5) the 2d dynamical system (NDIM $= 2$)

$$\begin{aligned} \dot{u}_1 &= Lu_2 \\ \dot{u}_2 &= \tfrac{L}{\kappa}\,[f'(u_1)\ - \mu]. \end{aligned} \tag{5.6}$$

where $L$ is the physical domain size, and dots and primes denote derivatives with respect to $\xi \equiv x/L$ and $\phi$, respectively. The advantage of this form is that the fields $u_1(\xi)$ and $u_2(\xi)$ correspond to the correctly scaled physical fields $\phi(L\xi)$ and $\partial_x\phi(L\xi)$. For simplicity, we use periodic boundary conditions for $u_1$ and $u_2$ (NBC $= 2$) that take the form

$$u_1(0) = u_1(1), \tag{5.7}$$
$$u_2(0) = u_2(1), \tag{5.8}$$

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

$$\int_0^1 (u_1 - \bar{\phi})\,\mathrm{d}\xi = 0. \tag{5.9}$$

As starting solution we use a small amplitude harmonic modulation of wavelength $L_c = 2\pi/k_c$ where $k_c = \sqrt{-f''(\phi_0)/\kappa}$ is the critical wavenumber for the linear instability of a uniform solution $\phi_0$. The starting solution has to fulfil the relation $\mu = f'(\phi_0)$ between $\mu$ and $\phi_0$.

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

There is a further complication as Eq. (5.6) corresponds to a conservative dynamical system (not a dissipative one). To deal with this we employ an 'unfolding parameter' $\epsilon$ that transforms the conservative into a 'virtual' dissipative system (with the same solutions). Different formulations are possible. Here we use:

$$\begin{aligned} \dot{u}_1 &= Lu_2 - \epsilon[f'(u_1)\ -\ \mu] \\ \dot{u}_2 &= L\,[f'(u_1)\ -\ \mu]/\kappa. \end{aligned} \tag{5.10}$$

The technique is mentioned in the auto07p demo `r3b` [2]) and further explained in Refs. [3, 4, 5]. It corresponds to the introduction of an unfolding term that embeds the conservative system into a one-parameter family of dissipative systems. Thereby the unfolding parameter $\epsilon$ creates a one-parameter family of solutions. Periodic solutions only exist for $\epsilon = 0$.

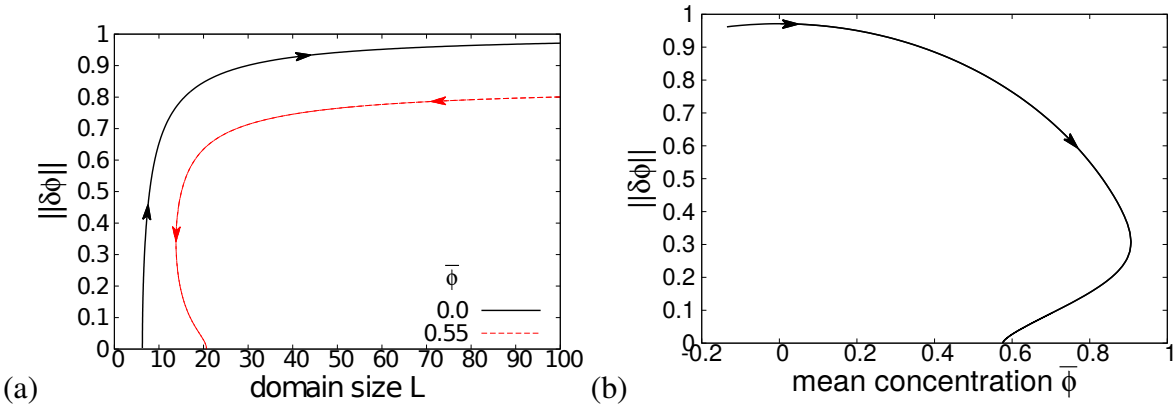


**Figure 5.1:** Graphic representation of the of dependencies of the norm $||\delta\phi|| = \sqrt{\int(\phi(x)-\bar{\phi})^2 dx}/L^{1/2}$ of periodic steady states on (a) domain size $L$ (PAR(5)) at $\bar{\phi} = 0$ and $\bar{\phi} = 0.55$, and (b) $\bar{\phi}$ (PAR(1))at $L = 100$ as obtained in (a) runs 1 and 111, and (b) run 11. Panel (a) shows cases of sub- and supercritical primary bifurcations (pitchfork of revolution). Note that the shown norm $||\delta\phi|| = \sqrt{||\phi||^2 - \bar{\phi}^2}$ is in the .f90 file provided as PAR49; to calculate it, add it into ICP as additional parameter.

## 5.2 Runs:

| **Python interface command line** | **Terminal command line** |
|---|---|
| *auto* | |
| **run 1:** Determine steady solutions as a function of domain size $L$ (PAR5), starting at the critical $L_c$ with a small amplitude sinusoidal solution. Set $a = -1$, $b = 1$, $\kappa = 1$, and fix mean value to $\bar{\phi} = \phi_0 = 0$. Let $\mu$ (PAR6), $\epsilon$ (PAR2) adapt. One finds that the primary bifurcation is supercritical.<br>Compute the branch of periodic solutions for $\phi_0 = 0$, continue in $L$ (PAR(5)) up to $L = 100$.<br>**Remaining true continuation parameters:** $\mu$ (PAR(6)) and $\epsilon$ (PAR(2));<br>**Parameters:** IPS$= 4$, ISP$= 0$, ISW$= 1$, ICP$= [5, 6, 2]$,<br>Start data from function *stpnt* (IRS$= 0$)<br>save output-files as `b.d1, s.d1, d.d1` | |
| *r1 = run(e = 'acch', c = 'acch.1', sv = 'acch1')* | *@@R acch 1*<br>*@sv d1* |
| **run 11:** Restart at domain size $L = 100$, change mean value $\bar{\phi}$ (PAR1), let $\mu$ (PAR6), $\epsilon$ (PAR2) adapt.<br>Continue in mean value $\bar{\phi}$ (PAR(1)) up to $\bar{\phi} = 1$, at fixed $L = 100$.<br>**Remaining true continuation parameters:** $\mu$ (PAR(6)) and $\epsilon$ (PAR(2))<br>**Other output:** as in run 1<br>**Parameters:** IPS$= 4$, ISP$= 0$, ISW$= 1$, ICP$= [1, 6, 2]$,<br>Start at final result of run 1: IRS$= 5$<br>save output-files as `b.d11, s.d11, d.d11` | |
| *r11 = run('acch1', e = 'acch', c = 'acch.11', sv = 'acch11')* | *@@R acch 11 d1*<br>*@sv d11* |

| | |
|---|---|
| **run 111:** Restart at $\bar{\phi} = 0.55$ (LAB9 of run 11), decrease domain size $L$ (PAR5), Let $\mu$ (PAR6), $\epsilon$ (PAR2) adapt. One finds that the primary bifurcation is subcritical.<br>Fix $\bar{\phi} = 0.55$, continue in $L$ (PAR(5)): decrease from $L = 100$. Stop at $L = 100$<br>**Remaining true continuation parameters:** $\mu$ (PAR(6)) and $\epsilon$ (PAR(2))<br>**Other output:** as in run 1<br>**Parameter:** IPS$= 4$, ISP$= 0$, ISW$= 1$, ICP$= [5, 6, 2]$,<br>Start at LAB9 of run 11: IRS$= 9$<br>save output-files as `b.d111, s.d111, d.d111` | |
| *r111 = run('acch11', e = 'acch', c = 'acch.111', sv = 'acch111')* | *@@R acch 111 d11*<br>*@sv d111* |
| **run 2:** As run 1, but with additional user-defined output, see Remarks.<br>Compute the branch of periodic solutions for $\phi_0 = 0$,<br>Continue in $L$ (PAR(5)) up to $L = 100$.<br>**Remaining true continuation parameters:** $\mu$ (PAR(6)) and $\epsilon$ (PAR(2));<br>**Other output:** amplitude (PAR46), largest slope (PAR48), $2^{\text{nd}}$ norm (PAR49)<br>**Parameter:** IPS$= 4$, ISP$= 0$, ISW$= 1$, ICP$= [5, 6, 2]$,<br>Start data from function *stpnt* (IRS$= 0$)<br>save output-files as `b.d2, s.d2, d.d2` | |
| *r2 = run(e = 'acch', c = 'acch.2', sv = 'acch2')* | *@@R acch 2*<br>*@sv d2* |
| *clean()* | *@cl* |

**Table 5.1:** Commands for running demo `acch`.

## 5.3 Remarks:

- The f90 file provides another integral condition that is not used in the demo. If used it allows for a determination of the energy of the obtained steady state solutions and therefore for a better interpretation of the physical meaning of the individual solutions found.
- 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. An example is run 2, that corresponds to run 1 with additional output of solution amplitude (PAR46), largest slope of solution (PAR48), and the norm of $\phi - \bar{\phi}$ (PAR49). To distinguish proper continuation parameters from other output parameters in ICP it is recommendable to separate them by several additional spaces (see file c.acch.2)
- Screen output and command line commands are provided in README file.

## 5.4 Tasks:

After running the examples, try to implement your own adaptations, e.g., do the following runs:

**3, 31, 311, 312** Activate the additional integral condition to measure the energy of the solutions [set

NINT=3 in the c.-file and include PAR9 as additional proper continuation parameter in ICP in the c.-file]. Redo runs 1, 11, 111, 112.

**4** Redo run 3 for other values of $\phi_0$, e.g., 0.25, -0.25, 0.5, 0.56, 0.7. [You have to change the value of MEANPHI in the routine STPNT in the f90 file) What do you observe? (There might be values where it does not work. Look at the norm and at the energy. If you find multiple solutions at identical parameter values reflect about their physical significance.

**5** Start at $\phi_0 = \bar{\phi} = 0$ (as in the initial run 1) but keep the domain size $L$ (PAR5) fixed. Instead continue in $\bar{\phi}$ (PAR1) and let $\mu$ (PAR6), $\epsilon$ (PAR2) adapt. Do this with other $\phi_0$, e.g., 0.25, -0.25, 0.5, 0.56, 0.7. Do you see differences to runs 4? [Remark: if the run does not start properly, use a small non-zero $\bar{\phi}$

**6** Run a continuation with fixed $\mu$ (you need to allow another parameter to adapt, e.g., $\bar{\phi}$). Compare your results with the ones obtained at fixed $\bar{\phi}$.

- Replace the used double-well potential by a different function e.g. the full Flory-Huggins energy.

## References

[1] 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.

[2] 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.

[3] E. J. Doedel et al. "Computation of periodic solutions of conservative systems with application to the 3-body problem". In: *Int. J. Bifurcation Chaos* 13 (2003), pp. 1353–1381. DOI: 10.1142/S0218127403007291.

[4] FJ Munoz-Almaraz et al. "Continuation of periodic orbits in conservative and Hamiltonian systems". In: *Physica D* 181 (2003), pp. 1–38. DOI: 10.1016/S0167-2789(03)00097-6.

[5] FJ Munoz-Almaraz et al. "Continuation of normal doubly symmetric orbits in conservative reversible systems". In: *Celest. Mech. Dyn. Astron.* 97 (2007), pp. 17–47. DOI: 10.1007/s10569-006-9048-3.