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Continuation

CHBC: Steady states of Cahn-Hilliard equation in confined geometry with energy bias

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7 chbc: Steady states of Cahn-Hilliard equation in confined geometry with energy bias

The tutorial CHBC explores steady solutions to the Cahn-Hilliard equation with imposed non-periodic boundary conditions (energetic bias). You will calculate steady solutions on different branches continuing them in the energetic bias parameter.

7.1 Model

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

$$\partial_t \phi = M \partial_{xx} \frac{\delta F}{\delta \phi} = -M \partial_{xx} [\kappa \partial_{xx} \phi - \partial_\phi f(\phi)] \quad (7.1)$$

where M is a constant mobility factor (not relevant for steady states), $\phi(x, t)$ is the independent (field) variable, μ is a parameter that stands for a chemical potential or Lagrange multiplier. In contrast to the demo `acch` [1] a finite domain $[0, L]$ without periodic boundary conditions (BC) is used and an energetic bias at the boundaries results in boundary conditions that differ (in general) from the periodic ones in the demo `acch` [1].

We use the free energy functional

$$F[\phi] = \int_L dx \left[\frac{\kappa}{2} (\partial_x \phi)^2 + f(\phi) \right] + a_m \phi_m + a_p \phi_p. \quad (7.2)$$

where the last two terms are boundary terms with $\phi_m = \phi(0)$ and $\phi_p = \phi(L)$. For background information regarding the Cahn-Hilliard equation see [2]. Similar one-dimensional profiles under energetic bias at the boundaries are discussed in the result section of [3].

For $f(\phi)$ we use as in the tutorial `acch` [1] the simple double well potential

$$f(\phi) = \frac{a}{2} \phi^2 + \frac{b}{4} \phi^4. \quad (7.3)$$

Remember, that the parameter $b > 0$ and a is arbitrary. The critical point is at $a = a_c = 0$.

The steady solutions fulfil

$$0 = \kappa \partial_{xx} \phi - \partial_\phi f(\phi) + \mu. \quad (7.4)$$

with boundary conditions

$$\partial_x \phi = a_m \quad \text{at} \quad x = 0, \quad (7.5)$$

$$\partial_x \phi = -a_p \quad \text{at} \quad x = L. \quad (7.6)$$

In the present runs we keep $\bar{\phi}$ fixed, i.e., μ takes the role of a Lagrange multiplier for the conservation of ϕ .

To use the continuation toolbox `auto07p`, we first write (7.4) as a system of first-order autonomous ordinary differential equations on the interval $[0, 1]$. To do so, we introduce the

variables $u_1 = \phi - \bar{\phi}$ and $u_2 = d\phi/dx$, and obtain from equation (7.4) the 2d dynamical system (NDIM = 2)

$$\begin{aligned} \dot{u}_1 &= Lu_2 \\ \dot{u}_2 &= \frac{L}{\kappa} [f'(u_1 + \bar{\phi}) - \mu]. \end{aligned} \quad (7.7)$$

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 this form is that the fields $u_1(\xi)$ and $u_2(\xi)$ correspond to the correctly scaled physical fields $\phi(L\xi)$ and $\partial_x\phi(L\xi)$. The two boundary conditions (NBC = 2) take the form

$$u_2(0) = a_m, \quad (7.8)$$

$$u_2(1) = -a_p. \quad (7.9)$$

Here, no integral conditions for computational pinning is needed as the BC already break the translational symmetry that the bulk equation has. However, we use the integral condition

$$\int_0^1 u_1 d\xi = 0. \quad (7.10)$$

for volume conservation and another one to calculate the bulk energy (NINT = 2).

As starting solution we use the trivial solution $u_1 = u_2 = 0$ for some particular domain size L . The starting solution has to fulfil the relation $\mu = f'(\bar{\phi})$ between μ and $\bar{\phi}$.

The number of free (continuation) parameters is given by NCONT = NBC+NINT-NDIM+1 and is here equal to 3. However, the third of them is the bulk energy that is calculated via the trick of an additional integral condition.

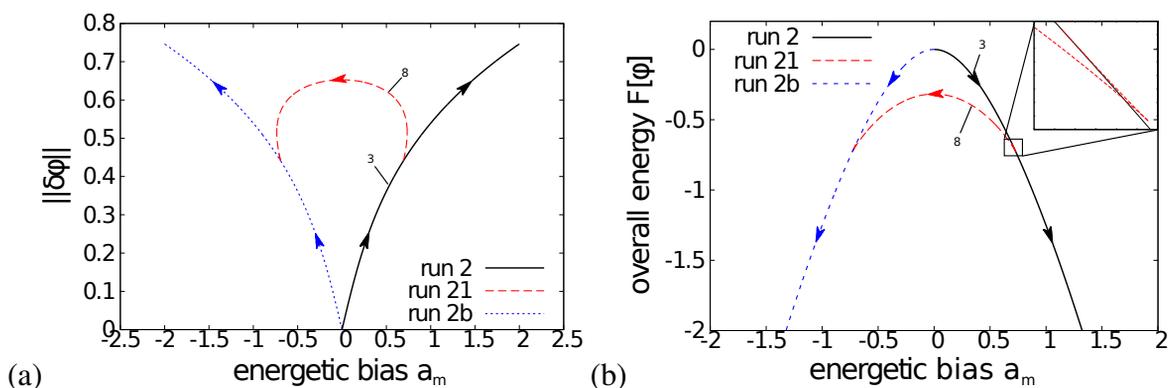


Figure 7.1: Graphic representation of (a) the norm $\|\delta\phi\| = \sqrt{(1/L) \int (\phi(x) - \bar{\phi})^2 dx}$ and (b) the overall energy [Eq. (7.2)] (PAR(47)) of steady states in dependence of the bias strength a_m (PAR(7)) in the case of symmetric bias $a_p = a_m$. The inset shows that the bifurcation is subcritical. The domain size is $L = 5$ and $\bar{\phi} = 0$ is fixed. The results are obtained in runs 2, 21, and 2b.

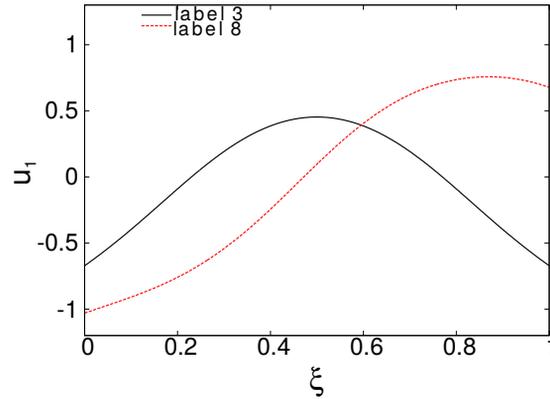


Figure 7.2: Solutions $u_1(\xi) = \phi - \bar{\phi}$ corresponding to symbols in Fig. 7.1

7.2 Runs:

Python interface command line	Terminal command line
<i>auto</i>	
<p>run 1: Determine steady solutions as a function of energetic bias a_m (PAR7) ($a_p = a_m$: symmetric case, fixed in f90 file) starting at trivial homogeneous state for $L = 5$. Set $a = -1$, $b = 1$, $\kappa = 1$, and fix mean value to $\bar{\phi} = 0$. Let μ (PAR6) and bulk energy (PAR9) adapt. One finds that enrichment layers form at the boundaries, but not much else happens. Compute the branch with increasing bias a_m, continue in a_m (PAR(7)) up to $a_m = 2$. Remaining true continuation parameters: μ (PAR(6)) and F_{bulk} (PAR(9)) Other output: boundary and overall energy (PAR(46) and PAR(47)) Parameter: IPS= 4, ISP= 0, ISW= 1, ICP= [7, 6, 9, 46, 47] Start data from function <i>stpnt</i> (IRS= 0) Save output-files as <i>b.r1</i>, <i>s.r1</i>, <i>d.r1</i></p>	
<i>r1 = run(e = 'chbc', c = 'chbc.1', sv = 'r1')</i>	<i>@@R chbc 1</i> <i>@sv r1</i>
<p>run 2: Same as run 1, but now detection of branching points is switched on (ISP=2 in c.file). One branching point detected. Save output-files as <i>b.r2</i>, <i>s.r2</i>, <i>d.r2</i></p>	
<i>r2 = run(e = 'chbc', c = 'ch.2', sv = 'r2')</i>	<i>@@R chbc 2</i> <i>@sv r2</i>
<p>run 21: Restart at branching point (LAB4 of run 2), switch branches (ISW=-1), continue in energetic boundary bias a_m (PAR7), let μ (PAR6) and bulk energy (PAR9) adapt. Another branching point and several folds are detected. If one lets the run go on long enough the continuation repeatedly follows a loop. Otherwise same as run 2. Save output-files as <i>b.r21</i>, <i>s.r21</i>, <i>d.r21</i></p>	
<i>r21 = run('r2', e = 'chbc', c = 'chbc.21', sv = 'r21')</i>	<i>@@R chbc 21 r2</i> <i>@sv r21</i>

run 2b: As run 2, but going backwards (towards negative a_m). Continue in $a_m < 0$ (PAR(7)). set DS= -0.001. Otherwise same as run 2. Save output-files as b.r2b, s.r2b, d.r2b	
<code>r2b = run(e = 'chbc', c = 'chbc.2b', sv = 'r2b')</code>	<code>@@R chbc 2b</code> <code>@sv r2b</code>
<code>clean()</code>	<code>@cl</code>

Table 7.1: Commands for running demo CHBC.

7.3 Remarks:

- Beside the NCONT true continuation parameters that have to be given as ICP in the c.-parameter file, we list other output parameters as defined in the subroutine PVLS in the f90 file. In particular, we show the boundary terms of the energy (PAR46) and the overall energy (PAR47). To distinguish proper continuation parameters from other output parameters in ICP it is recommendable to separate them by several additional spaces.
- Screen output and command line commands are provided in README file. The results are presented in Fig. 7.1.

7.4 Tasks:

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

- Determine the complete bifurcation diagram for different domain sizes: $L = 3.5$ and $L = 10$. Seeing the result for $L = 10$ do you dare to try $L = 25$? Can you explain the symmetry of the bifurcation diagram?
- Change $\bar{\phi}$ and repeat the runs, e.g., use 0.25, -0.25, 0.5, 0.56, 0.7. What overall changes to the bifurcation diagram do you observe? Why does this happen? [try $L = 5$ first]
- In the f90 file you can switch from the symmetrical case ($a_p = a_m$), to the antisymmetrical case ($a_p = -a_m$) or the asymmetrical case ($a_p = 0$). This is already prepared, you only need to comment/uncomment the appropriate lines in the subroutines BCND and PVLS. You can play around with this and observe what happens to the symmetries of the bifurcation diagram.

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] U. Thiele, S. Madruga, and L. Frastia. “Decomposition driven interface evolution for layers of binary mixtures: I. Model derivation and stratified base states”. In: *Phys. Fluids* 19 (2007), p. 122106. DOI: [10.1063/1.2824404](https://doi.org/10.1063/1.2824404).