Validated Saddle-Node Bifurcations and Applications to Lattice Dynamical Systems

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Introduction to the Discrete Allen-Cahn Equation

Allen-Cahn Equation: fundamental model for interface motion during solidification in two-phase materials

$$u_t = \Delta u + \lambda f(u), u_x(t,0) = u_x(t,1) = 0$$

It cannot explain the pinning of fronts, i.e., fronts which get stuck and stop moving as time increases

Spatially discrete Allen-Cahn Equation
Cahn, Chow, Grant, Mallet-Paret, Van Vleck 1995-6

Somewhat intractable, requires special nonlinearities

Our work: develop bifurcation tools for computer validation, rigorously prove statements about the nature of solutions.

Parameters and Equilibria

Spatially Discrete Allen-Cahn

$$\dot{u}_k = u_{k+1} - 2u_k + u_{k-1} + \lambda f(u_k)$$

$$\text{Boundary Conditions: } u_0 = u_1 \;,\; u_{n+1} = u_n$$

$$\text{Our Nonlinearity: } f(u) = \left(1 - u^2\right)(u - \mu)$$

Parameters:

- Fixed mass $\mu \in (-1, 1)$ (mostly $\mu = 0$)
- Bifurcation parameter λ, $1/\sqrt{\lambda}$ = interaction length

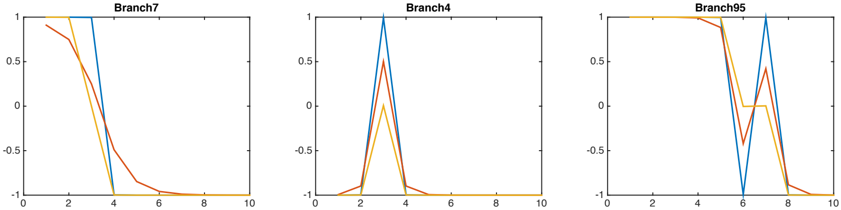
Mosaic solutions: For large λ

- exactly 3^n equilibria $u_k \approx 0, \pm 1$ – cause pinning
- 2^n equilibria are stable, $u_k \approx \pm 1$

Mosaic solutions for $n = 10$

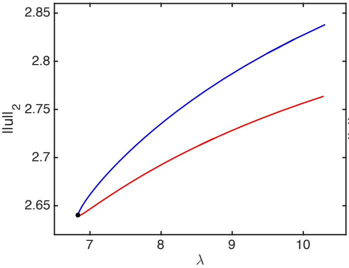
Binary notation: Denote each stable mosaic solution in binary e.g. $7 = 1 \cdot 2^0 + 1 \cdot 2^1 + 1 \cdot 2^2$ shown for $\lambda = 300$ blue

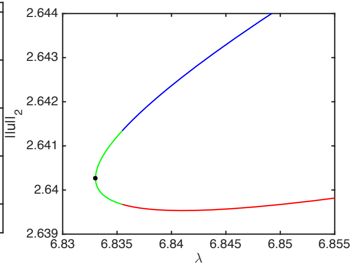
Grain: Consecutive set with no change in sign. Solution 7 has minimum grain size 3 and number of grains 2.



Mosaic solutions for $n = 10$

Bifurcation: Since there are no stable equilibria for $\lambda \approx 0$





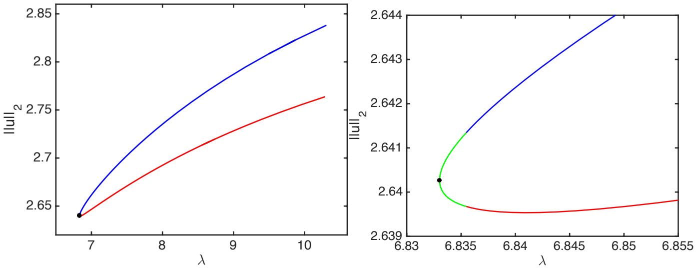
Mosaic solutions for $n = 10$

Bifurcation: Since there are no stable equilibria for $\lambda \approx 0$

Validation: 960 saddle-node bifurcations (out of 1022)

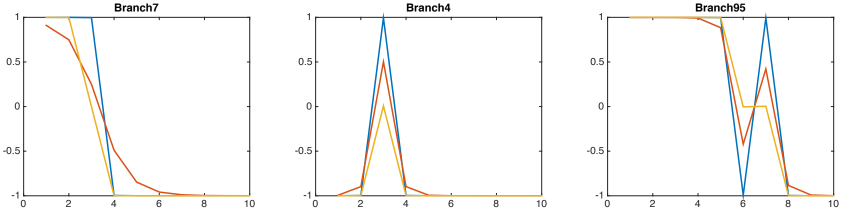
We can actually validate the entire branch $\lambda \to \infty$

Many of the rest are pitchfork bifurcations, not necessarily at the bifurcation point, but we cannot validate the entire branch



Mosaic solutions for $n = 10$

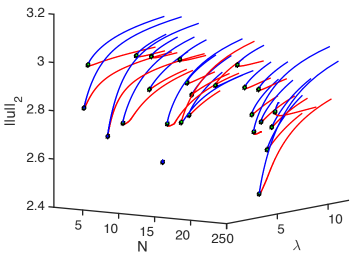
Color coding: At bifurcation Unstable equilibrium at $\lambda = 300$

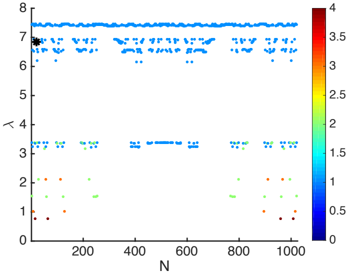


Robustness of Grains for $n = 10$

Grant showed that for a different special nonlinearity, grain size is related to robustness

Color indicates grain size





Validation of Robustness of Grains for $n = 10$

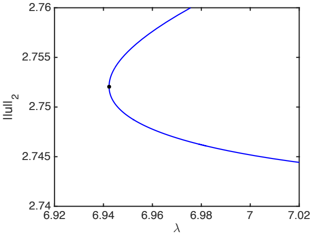
Theorem (Grain size and robustness)

Let u denote a stable mosaic solution of the discrete Allen-Cahn Equation with $\mu = 0$ and $n = 10$, and let $\lambda_0(u)$ denote the parameter value of the associated saddle-node bifurcation.

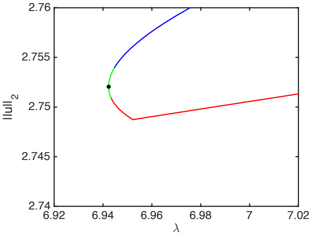
- *If $\lambda_0 < 3$, then the size of the smallest grain is greater than 1 and the number of grains is equal to 2 or 3.*
- *If $\lambda_0 > 3.5$, then the size of the smallest grain is equal to 1 and the number of grains is at least 3.*

In addition to this theorem, we make a number of observations on robustness questions.

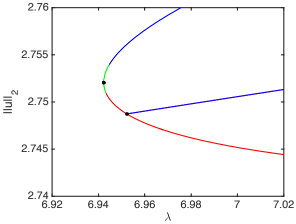
Validation Corrects Numerical Errors: Branch 40



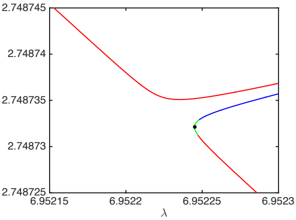
What AUTO thinks it sees



What validation proves

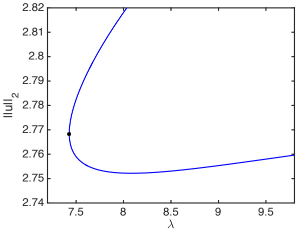


What multiple validations prove

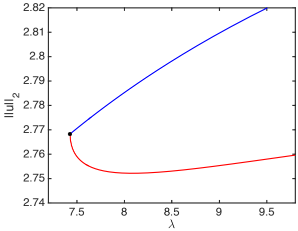


What it really does

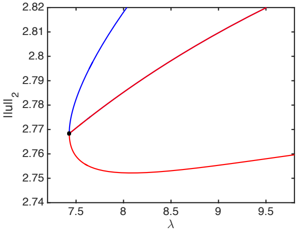
Validation Corrects Numerical Errors: Branch 144



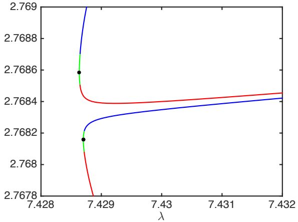
What AUTO thinks it sees



What validation proves



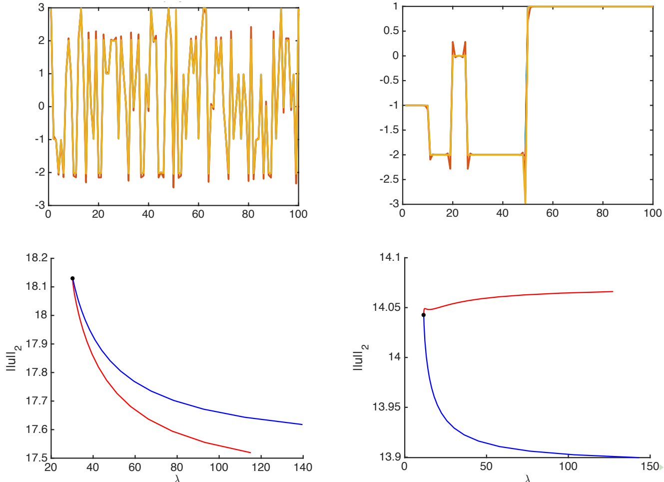
What multiple validations prove



What it really does

Mosaic Solutions for $n = 100$

Our validation method is extremely flexible – with almost no changes, we can validate for a 100-dimensional system with a new nonlinearity: $f(u) = \sin(\pi u)/\pi$.



The constructive implicit function theorem

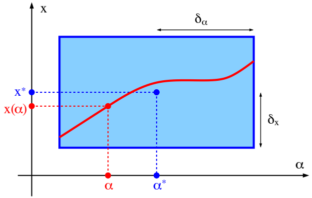
In Banach spaces, we seek a zero set of $G : P \times X \to Y$.

Assume

1. $\|G(\alpha^*, x^*)\|$ small (cf. equal to zero)
2. $\|D_x G(\alpha^*, x^*)\|$ bounded by a known value (cf. exists)
3. A Lipschitz condition on $D_x G$
4. A Lipschitz condition on $D_\alpha G$

then inside an explicit $(\delta_\alpha, \delta_x)$ box there is a unique smooth $x(\alpha)$ such that

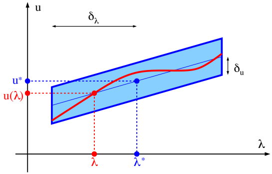
$$G(\alpha, x(\alpha)) = 0.$$

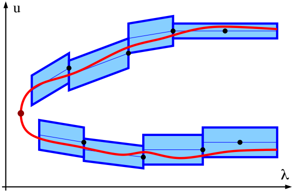


Proof via the contraction mapping principle

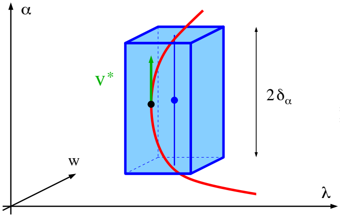
Extended to Multiple Boxes

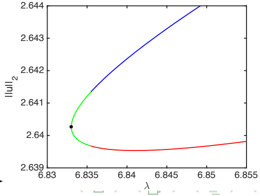
In order to perform continuation efficiently, we have extended to parallelograms, and to a chain, validating the whole curve.





We apply it to continue at saddle-node bifurcation points.





But How Can We Validate the Entire Branch?(1)

Our numerical validation also can be used analytically

For $\mu = 0$, $u^* \in \{-1, 0, 1\}^n$ fixed.
Consider a 0.1-neighborhood of u^*.

$$G(u) = \frac{1}{\lambda} Au + f(u) \ , \ f(u) = diag(u - u^3)$$

$$A = \begin{bmatrix} -1 & 1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & 1 & -2 & 1 \\ 0 & \cdots & 0 & 1 & -1 \end{bmatrix} \text{ implies } \|A\| \leq 4$$

But How Can We Validate the Entire Branch?(2)

Small residual for G:

$$G(u) = \frac{1}{\lambda} Au + f(u)$$

$$\|A\| \leq 4 \text{ and } f(u^*) = 0, \text{ and therefore}$$

$$\|G(u^*)\| \leq \frac{4}{\lambda}$$

But How Can We Validate the Entire Branch?(2)

Linear operator bound Assume that A is a bounded linear operator, and B is one-to-one and onto. If

$$\|I - BA\| \leq \rho_1 < 1 \qquad \text{and} \qquad \|B\| \leq \rho_2$$

then A^{-1} exists and

$$\|A^{-1}\| \leq \frac{\rho_2}{1-\rho_1}$$

But How Can We Validate the Entire Branch?(3)

Inverse bound on derivative:

$$D_u G(u^*) = \frac{1}{\lambda} A + diag(f'(u^*)) \; := \frac{1}{\lambda} A + B^{-1}$$

$$f'(u) = 1 - 3u^2 \text{ implies } \|B\| \leq 1$$

$$\|I - B\, D_u G(u^*)\| = \left\| I - \frac{1}{\lambda} BA - B \;\text{diag}(f'(u^*)) \right\| = \left\| \frac{BA}{\lambda} \right\| \leq \frac{4}{\lambda}$$

Using the linear operator bound

$$\|(D_u G(u^*))^{-1}\| < \frac{1}{1 - 4/\lambda}$$

But How Can We Validate the Entire Branch?(4)

Lipschitz derivative:

$$\begin{aligned} \|D_u G(u) - D_u G(u^*)\| &\leq \max_{|\xi| \leq \|u^*\| + 0.1} |f''(\xi)| \, \|u - u^*\| \\ &\leq 6(1 + 0.1) \, \|u - u^*\| \end{aligned}$$

But How Can We Validate the Entire Branch?(5)

Specific bounds in constructive implicit function theorem:

$$\frac{105.6\,\lambda}{(\lambda-4)^2} < 1 \qquad \text{and} \qquad \frac{8}{\lambda-4} < 0.1,$$

which hold for all $\lambda > 113.459$

This gives a uniqueness radius of ≈ 0.075

For all $\lambda > 114$, there is a unique mosaic solution within 0.075 of u^*, and no bifurcations can occur.

Summary

- Constructive implicit function theorem allows us to design a flexible validation technique for validating branches of solutions with saddle-node bifurcation
- For the discrete Allen-Cahn model, this provides a flexible method that can be adapted to related situations with little fuss. We produced results that could not have been done analytically, and detected errors from naive numerical methods.
- E.S. and Thomas Wanner, Validated Bifurcation Methods and Applications to Lattice Dynamical Systems, SIADS, 15-3 (2016) 1690-1733, DOI: 10.1137/16M1061011.
- Developed techniques for equivariant pitchfork bifurcations. J-P Lessard, E.S., and T. Wanner, Rigorous continuation of bifurcation points in the diblock copolymer equation, submitted.