Uncertainty quantification analysis of bifurcations of PDEs with random coefficients

Chiara Piazzola

joint with Christian Kuehn and Elisabeth Ullmann

Department of Mathematics
Technical University of Munich

November 12, 2024

Outline

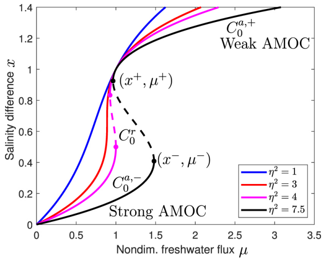
Outline

The Atlantic meridional overturning circulation (AMOC)

An ODE model[1]

Input parameters	→	Model	→	Output
(μ, η)		$\dot{x}(t) = \mathcal{M}(x(t), \eta(\omega))$		$x = x(t; \mu, \eta)$

- μ: bifurcation parameter
- (x, μ): **equilibria** of the system
- (x^-, μ^-) and (x^+, μ^+): **bifurcation/tipping points**
- The parameter η determines the overall qualitative behavior of the system



Equilibrium curves[1].

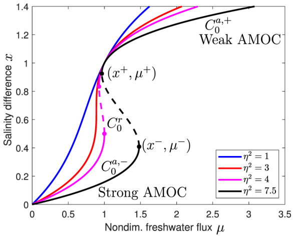
[1] K. Lux et al. "Assessing the impact of parametric uncertainty on tipping points of the Atlantic meridional overturning circulation". In: *Environmental Research Letters* (2022).

Uncertainty quantification analysis

$$\begin{array}{c} \text{Random parameters} \\ \eta(\omega) \text{ on } (\Omega, \mathcal{F}, \mathbb{P}) \end{array} \longrightarrow \begin{array}{c} \text{Model} \\ \dot{x}(t) = \mathcal{M}(x(t), \eta(\omega)) \end{array} \longrightarrow \begin{array}{c} \text{Output} \\ x = x(t, \omega) \end{array}$$

Uncertainty quantification analysis

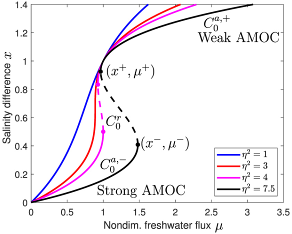
Random parameters $\eta(\omega)$ on $(\Omega, \mathcal{F}, \mathbb{P})$	→	Model $\dot{x}(t) = \mathcal{M}(x(t), \eta(\omega))$	→	Output $x = x(t, \omega)$



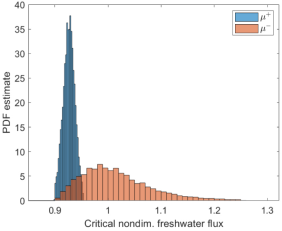
Equilibrium curves[1].

Uncertainty quantification analysis

Random parameters $\eta(\omega)$ on $(\Omega, \mathcal{F}, \mathbb{P})$	→	Model $\dot{x}(t) = \mathcal{M}(x(t), \eta(\omega))$	→	Output $x = x(t, \omega)$



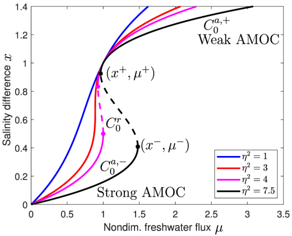
Equilibrium curves[1].



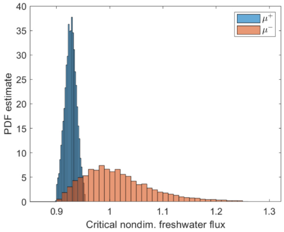
Distribution of $\mu^-(\omega), \mu^+(\omega)$[1].

Uncertainty quantification analysis

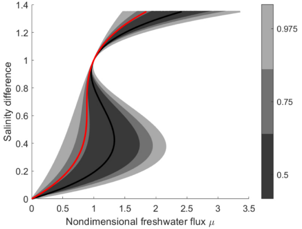
Random parameters $\eta(\omega)$ on $(\Omega, \mathcal{F}, \mathbb{P})$ → Model $\dot{x}(t) = \mathcal{M}(x(t), \eta(\omega))$ → Output $x = x(t, \omega)$



Equilibrium curves[1].



Distribution of $\mu^-(\omega), \mu^+(\omega)$[1].



Probabilistic bifurcation diagram[1].

Goal of this work

Uncertainty quantification analysis of bifurcations of PDEs with random coefficients:

Goal of this work

Uncertainty quantification analysis of bifurcations of PDEs with random coefficients:

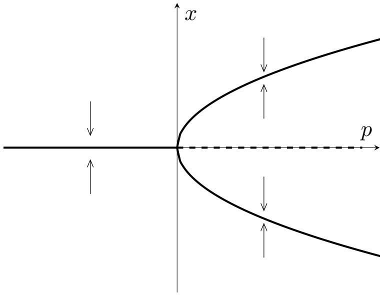
Supercritical pitchfork bifurcation

$$\dot{x} = px - x^3, \quad p \in \mathbb{R}$$

- Equilibria are solutions of $\dot{x} = 0$:

$$x^* = 0 \quad \text{and} \quad p - x^{*2} = 0$$

- $(0, 0)$ is the bifurcation point



Goal of this work

Uncertainty quantification analysis of bifurcations of PDEs with random coefficients:

Bifurcations	**Pitchfork type**
Reaction-diffusion equations with polynomial nonlinearity	**The Allen–Cahn equation**
What the impact of the randomness on the dynamics?	**Bifurcation theory**
How can we do UQ analysis in an efficient manner?	**Surrogate modeling**

The Allen–Cahn equation with random coefficients

$$
\begin{aligned}
\partial_t u &= \Delta u + q(\mathbf{x},\omega)u - u^3, && \mathbf{x} \in D \subset \mathbb{R}^d,\ d = 1, 2, 3, \\
u &= 0, && \mathbf{x} \in \partial D,\ \mathbb{P}\text{-almost surely},
\end{aligned}
$$

where

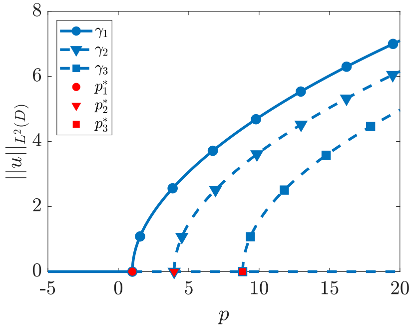
- $(\Omega, \mathcal{F}, \mathbb{P})$: probability space,
- $q(\mathbf{x},\omega) : \overline{D} \times \Omega \to \mathbb{R}$: random coefficient function,
- $u = u(t, \mathbf{x}, \omega)$: random solution.

Outline

The Allen–Cahn equation

$$\begin{aligned} \partial_t u &= \Delta u + pu - u^3, && \mathbf{x} \in D \subset \mathbb{R}^d,\ p \in \mathbb{R}, \\ u &= 0, && \mathbf{x} \in \partial D. \end{aligned}$$

- Equilibria are solutions of the stationary problem
  - Trivial branch: $\{(p, 0) \mid p \in \mathbb{R}\}$
  - Non-trivial branch: $\gamma_i = \{(p, u(p)) \mid p \geq p_i^*\}$
- Bifurcation points: $(p_i^*, 0)$
- Bifurcation parameter: $p \in \mathbb{R}$



The Allen–Cahn equation
Bifurcation analysis

Main tool to prove existence of pitchfork bifurcations: Crandall–Rabinowitz theorem[2].

Let $F(p,u) := \Delta u + pu - u^3$.

- Condition 1: failure of the implicit function theorem
  - $\mathrm{D}_u F(p,0)$ has a zero eigenvalue
  - Since $\mathrm{D}_u F(p,0)v = \Delta v + pv$, the bifurcation value is $p_i^* = -\lambda_i$
- Condition 2: bifurcation points correspond to simple eigenvalues of $\mathrm{D}_u F(p,0)$
- Local shape of bifurcation curves is inferred by computing higher order derivatives of F

[2] H. Kielhofer. *Bifurcation Theory: An Introduction with Applications to Partial Differential Equations*. Springer, 2014.

The Allen–Cahn equation with random coefficients

$$\begin{aligned} \partial_t u &= \Delta u + q(\mathbf{x},\omega)u - u^3, && \mathbf{x} \in D \subset \mathbb{R}^d,\ p \in \mathbb{R}, \\ u &= 0, && \mathbf{x} \in \partial D,\ \mathbb{P}\text{-almost surely}, \end{aligned}$$

where

- $(\Omega, \mathcal{F}, \mathbb{P})$: probability space,
- $q(\mathbf{x},\omega) : \overline{D} \times \Omega \to \mathbb{R}$: random coefficient function,
- $u = u(t, \mathbf{x}, \omega)$: random solution.

The Allen–Cahn equation with random coefficients

Assumption 1

We assume the random field $q(\mathbf{x}, \omega)$ to be of the following form

$$q(\mathbf{x}, \omega) = p + g(\mathbf{x}, \omega), \quad p \in \mathbb{R}$$

- $\mathbb{E}[g(\mathbf{x}, \omega)] = 0$, $\forall \mathbf{x} \in \overline{D}$,

The Allen–Cahn equation with random coefficients

Assumption 1

We assume the random field $q(\mathbf{x}, \omega)$ to be of the following form

$$q(\mathbf{x}, \omega) = p + g(\mathbf{x}, \omega), \quad p \in \mathbb{R}$$

- $\mathbb{E}[g(\mathbf{x}, \omega)] = 0$, $\forall \mathbf{x} \in \overline{D}$,

➙ Same structure as the classic AC with an additional linear term

➙ $\mathbb{E}[q(\mathbf{x}, \omega] = p$: bifurcation parameter is a hyper-parameter of the random field model

The Allen–Cahn equation with random coefficients

Assumption 1

We assume the random field $q(\mathbf{x},\omega)$ to be of the following form

$$q(\mathbf{x},\omega) = p + g(\mathbf{x},\omega), \quad p \in \mathbb{R}$$

- $\mathbb{E}[g(\mathbf{x},\omega)] = 0$, $\forall \mathbf{x} \in \overline{D}$,
- g is uniformly bounded: $\exists \bar{g} \in \mathbb{R}$ s.t. $\mathbb{P}(\omega \in \Omega : |g(\mathbf{x},\omega)| \leq \bar{g} \ \forall \mathbf{x} \in \overline{D}) = 1$,

→ Same structure as the classic AC with an additional linear term

→ $\mathbb{E}[q(\mathbf{x},\omega] = p$: bifurcation parameter is a hyper-parameter of the random field model

The Allen–Cahn equation with random coefficients

Assumption 2

We assume that the random field $g(\mathbf{x}, \omega)$ is parametrized by a finite number N of independent random variables $Y_n(\omega)$, $n = 1, \dots, N$ with $\mathbf{Y}(\omega) = [Y_1(\omega), \dots, Y_N(\omega)]$ such that

- $\mathbf{Y} : \Omega \to \Gamma$, $\omega \mapsto \mathbf{y} = [y_1, \dots, y_N]$,
- $\rho : \Gamma \to \mathbb{R}_+$, $\rho(\mathbf{y}) = \prod_{i=1}^{N} \rho_i(y_i)$: joint probability density function.

The Allen–Cahn equation with random coefficients

Assumption 2

We assume that the random field $g(\mathbf{x}, \omega)$ is parametrized by a finite number N of independent random variables $Y_n(\omega)$, $n = 1, \dots, N$ with $\mathbf{Y}(\omega) = [Y_1(\omega), \dots, Y_N(\omega)]$ such that

- $\mathbf{Y} : \Omega \to \Gamma$, $\omega \mapsto \mathbf{y} = [y_1, \dots, y_N]$,
- $\rho : \Gamma \to \mathbb{R}_+$, $\rho(\mathbf{y}) = \prod_{i=1}^{N} \rho_i(y_i)$: joint probability density function.

➙ The AC with random coefficients is now posed on the finite-dimensional probability space $(\Gamma, \mathcal{B}(\Gamma), \mathbb{P}_{\mathbf{Y}})$

➙ $g, u \colon \overline{D} \times \Gamma \to \mathbb{R}$

The Allen–Cahn equation with random coefficients

Bifurcation analysis

We turn the Allen–Cahn equation with random coefficients to the following parametric form

$$
\begin{aligned}
\Delta u + pu + g(\mathbf{x},\mathbf{y})u - u^3 &= 0, && \mathbf{x} \in D, \\
u &= 0, && \mathbf{x} \in \partial D,\ \mathbb{P}_{\mathbf{Y}} - \text{a.s.}.
\end{aligned}
$$

The Allen–Cahn equation with random coefficients
Bifurcation analysis

We turn the Allen–Cahn equation with random coefficients to the following parametric form

$$\begin{aligned} \Delta u + pu + g(\mathbf{x},\mathbf{y})u - u^3 &= 0, && \mathbf{x} \in D, \\ u &= 0, && \mathbf{x} \in \partial D, \ \mathbb{P}_{\mathbf{Y}} - \text{a.s.}. \end{aligned}$$

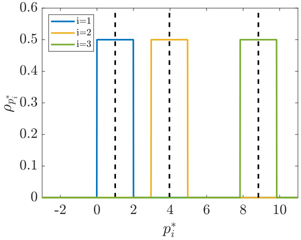
Bifurcation points: $(p_i^*(\mathbf{y}), 0)$

- $\widehat{F}(p,u) := \Delta u + pu + g(\mathbf{x},\mathbf{y})u - u^3$
- $\mathrm{D}_u \widehat{F}(p,0)v = \Delta v + pv + g(\mathbf{x},\mathbf{y})v$.
- $p_i^*(\mathbf{y}) = -\lambda_i^g(\mathbf{y})$, where λ_i^g is the ith-eigenvalue of $\Delta v + g(\mathbf{x},\mathbf{y})v$.

The Allen–Cahn equation with random coefficients
Bifurcation analysis

If $g(\mathbf{x}, \mathbf{y}) = g(\mathbf{y})$:

$$p_i^*(\mathbf{y}) = -\lambda_i - g(\mathbf{y})$$



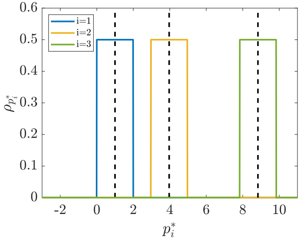
$g(x, y) = y$, $Y \sim$ Unif$[-1, 1]$

[3] A. Chernov and T. Lê. "Analytic and Gevrey Class Regularity for Parametric Elliptic Eigenvalue Problems and Applications". In: *SIAM Journal on Numerical Analysis* (2024)

The Allen–Cahn equation with random coefficients
Bifurcation analysis

If $g(\mathbf{x},\mathbf{y}) = g(\mathbf{y})$:

$$p_i^*(\mathbf{y}) = -\lambda_i - g(\mathbf{y})$$



$g(x,y) = y$, $Y \sim$ Unif$[-1,1]$

In general:

Proposition

If g is $\mathbf{y}-$analytic, the bifurcation values arising in correspondence of a simple eigenvalue are realizations of an associated random variable $p_i^*(\mathbf{Y})$.

It follows from the analyticity of such eigenvalues[3].

[3] A. Chernov and T. Lê. "Analytic and Gevrey Class Regularity for Parametric Elliptic Eigenvalue Problems and Applications". In: *SIAM Journal on Numerical Analysis* (2024)

The Allen–Cahn equation with random coefficients

Bifurcation analysis

Non-trivial branches of equilibria: $\gamma(\mathbf{y}) = \{(p, u(p, \mathbf{y})) \,|\, p \geq p^*(\mathbf{y})\}$

The Allen–Cahn equation with random coefficients

Bifurcation analysis

Non-trivial branches of equilibria: $\gamma(\mathbf{y}) = \{(p, u(p, \mathbf{y})) \,|\, p \geq p^*(\mathbf{y})\}$

- For $\mathbf{y} \in \Gamma$ fixed, derivatives of $\widehat{F}(p, u)$ looks similar to the classic case. We conclude that the bifurcations are of type supercritical pitchfork.

The Allen–Cahn equation with random coefficients
Bifurcation analysis

Non-trivial branches of equilibria: $\gamma(\mathbf{y}) = \{(p, u(p, \mathbf{y})) \,|\, p \geq p^*(\mathbf{y})\}$

- For $\mathbf{y} \in \Gamma$ fixed, derivatives of $\widehat{F}(p, u)$ looks similar to the classic case. We conclude that the bifurcations are of type supercritical pitchfork.

- Let $\mathbf{y} \in \Gamma$ be fixed. Then the curve $\gamma(\mathbf{y})$ can be parametrized as follows

$$\gamma(\mathbf{y}) = \{(r(s, \mathbf{y}), u(s, \mathbf{y})) \,|\, s \in [0, S], (r(0, \mathbf{y}), u(0, \mathbf{y})) = (p^*(\mathbf{y}), 0)\}$$

$$\{\gamma(s, \mathbf{Y})\}_{s \in [0,S]} = \{(r(s, \mathbf{Y}), u(s, \mathbf{Y}))\}_{s \in [0,S]} \quad \text{random parametrized curve}$$

The Allen–Cahn equation with random coefficients
Bifurcation analysis

Non-trivial branches of equilibria: $\gamma(\mathbf{y}) = \{(p, u(p, \mathbf{y})) \,|\, p \geq p^*(\mathbf{y})\}$

- For $\mathbf{y} \in \Gamma$ fixed, derivatives of $\widehat{F}(p, u)$ looks similar to the classic case. We conclude that the bifurcations are of type supercritical pitchfork.

- Let $\mathbf{y} \in \Gamma$ be fixed. Then the curve $\gamma(\mathbf{y})$ can be parametrized as follows

$$\gamma(\mathbf{y}) = \{(r(s, \mathbf{y}), u(s, \mathbf{y})) \,|\, s \in [0, S], (r(0, \mathbf{y}), u(0, \mathbf{y})) = (p^*(\mathbf{y}), 0)\}$$

$$\{\gamma(s, \mathbf{Y})\}_{s\in[0,S]} = \{(r(s, \mathbf{Y}), u(s, \mathbf{Y}))\}_{s\in[0,S]} \quad \text{random parametrized curve}$$

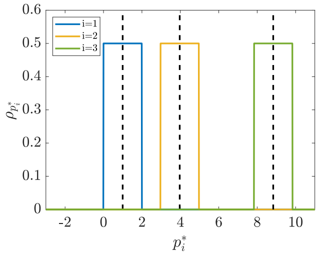
- Mean bifurcation curve:

$$\overline{\gamma}_i : \; = \{(\bar{r}(s), \bar{u}(s)) = (\mathbb{E}[r(s, \mathbf{Y})], \mathbb{E}[u(s, \mathbf{Y})]) \,,\, s \in [0, S], (\bar{r}(0), \bar{u}(0)) = (\mathbb{E}[p_i^*(\mathbf{Y})], 0)\}$$

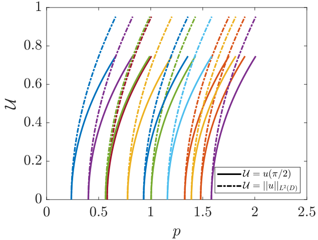
The Allen–Cahn equation with random coefficients

Spatially-homogeneous coefficients

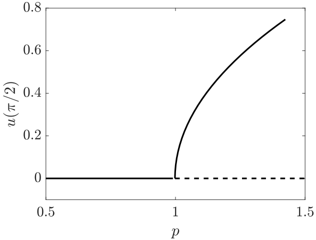
We consider the 1d Allen–Cahn equation on $D = [0, \pi]$ with $g(x, y) = y$, $Y \sim$ Unif$[-1, 1]$.



Pdf of p_i^*



Samples of $\gamma_1(Y)$



Mean bifurcation diagram

Outline

The Polynomial Chaos expansion[4]

Bifurcation points:

$$p_i^*(\mathbf{Y}) \qquad\qquad p_i^*(\mathbf{y}) \approx p^*_{\mathsf{PC}}(\mathbf{y}) = \sum_{\boldsymbol{\alpha}\in\Lambda} \widehat{p^*_{\boldsymbol{\alpha}}}\psi_{\boldsymbol{\alpha}}(\mathbf{y})$$

Bifurcation curves:

$$r(s,\mathbf{y}) \approx r_{\mathsf{PC}}(s,\mathbf{y}) := \sum_{\boldsymbol{\alpha}\in\Lambda} \widehat{r}_{\boldsymbol{\alpha}}(s)\psi_{\boldsymbol{\alpha}}(\mathbf{y}),$$

$$\{(r(s,\mathbf{Y}), u(s,\mathbf{Y}))\}\,,\ s \text{ fixed} \qquad\qquad u(r,\mathbf{y}) \approx u_{\mathsf{PC}}(s,\mathbf{y}) := \sum_{\boldsymbol{\alpha}\in\Lambda} \widehat{u}_{\boldsymbol{\alpha}}(s)\psi_{\boldsymbol{\alpha}}(\mathbf{y})$$

where $\psi_{\boldsymbol{\alpha}}$ are $\rho(\mathbf{y})\mathrm{d}\mathbf{y}$-orthonormal multivariate polynomials of degree α_n in the variable y_n and $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_N) \in \mathbb{N}^N_{\geq 0}$.

[4] D. Xiu and G. E. Karniadakis. "The Wiener–Askey Polynomial Chaos for Stochastic Differential Equations". In: *SIAM Journal on Scientific Computing* (2002)

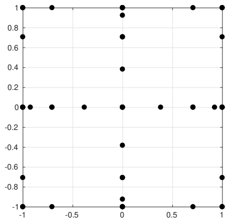
The PC expansion

❖ Which family of polynomials?

- Legendre polynomials for uniform random variables
- ...

❖ How to compute the coefficients? Stochastic collocation

- Set of collocation points $\rightarrow$ sparse grid
- Type of points chosen according to the distribution of $\mathbf{Y}$
  - Uniform r.v.: Gauss–Legendre, Leja, Clenshaw–Curtis, ...
  - ...
- Convert the sparse-grids-based Lagrange approximation to a PC approximation



The PC expansion: bifurcation points[5]

$$\text{Bifurcation points: } p_i^*(\mathbf{Y}) \quad \rightarrow \quad p_1^*(\mathbf{y}) \approx p_{\mathsf{PC}}^*(\mathbf{y}) = \sum_{\boldsymbol{\alpha}\in\Lambda} \widehat{p_{\boldsymbol{\alpha}}^*}\psi_{\boldsymbol{\alpha}}(\mathbf{y})$$

➙ Solve a set of independent deterministic eigenvalue problems at the collocation points.

- Remember that $p_i^*(\mathbf{y}) = -\lambda_i^g(\mathbf{y})$

[5] B. Sousedík et al. "On surrogate learning for linear stability assessment of Navier-Stokes Equations with stochastic viscosity". In: *Applications of Mathematics* (2022)

The PC expansion: bifurcation curves

Bifurcation curves:

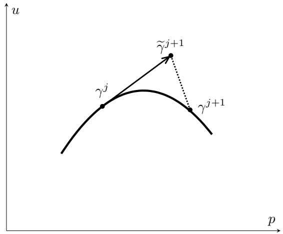
$$\{(r(s,\mathbf{Y}), u(s,\mathbf{Y}))\}, \; s \text{ fixed}$$

$$r(s,\mathbf{y}) \approx r_{\mathsf{PC}}(s,\mathbf{y}) := \sum_{\boldsymbol{\alpha}\in\Lambda} \widehat{r}_{\boldsymbol{\alpha}}(s)\psi_{\boldsymbol{\alpha}}(\mathbf{y}),$$

$$u(r,\mathbf{y}) \approx u_{\mathsf{PC}}(s,\mathbf{y}) := \sum_{\boldsymbol{\alpha}\in\Lambda} \widehat{u}_{\boldsymbol{\alpha}}(s)\psi_{\boldsymbol{\alpha}}(\mathbf{y})$$

➙ Approximate a set of independent deterministic branches arising at the collocation points.

- We need to solve a parametric nonlinear root-finding problem
- Numerical continuation
- s is the pseudo-arclength parameter



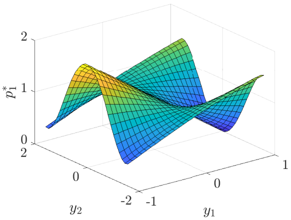
Implementation

- PC expansion: The Sparse Grids Matlab Kit
  - `https://github.com/lorenzo-tamellini/sparse-grids-matlab-kit`
  - C. Piazzola and L. Tamellini. “Algorithm 1040: The Sparse Grids Matlab Kit - a Matlab implementation of sparse grids for high-dimensional function approximation and uncertainty quantification”. In: *ACM Transactions on Mathematical Software* (2024)

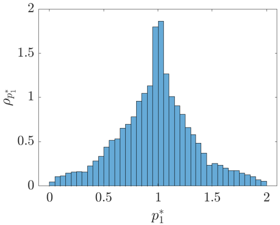
- Numerical continuation solver: Continuation Core and Toolboxes (COCO)
  - `https://sourceforge.net/projects/cocotools/`
  - H. Dankowicz and F. Schilder. *Recipes for Continuation*. Society for Industrial and Applied Mathematics, 2013

Numerical results
Bifurcation points

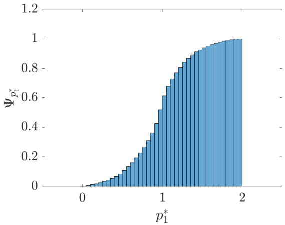
We consider the 1d Allen–Cahn equation on $D = [0, \pi]$ with $g(x, \mathbf{Y}) = Y_1 \cos(Y_2\, x)$, where $Y_1 \sim U([-1, 1])$, $Y_2 \sim U([-\pi/2, \pi/2])$.



gPC approximation of p_1^*



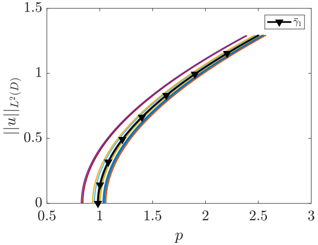
Pdf of p_1^*



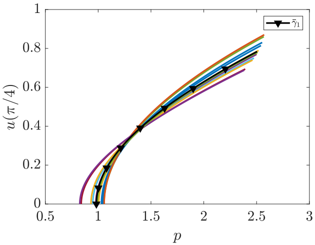
Cdf of p_1^*

Numerical results

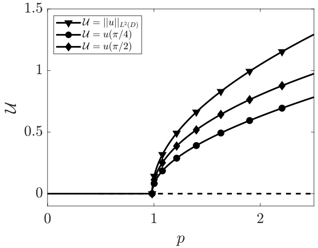
Bifurcation curves



Realizations and mean branch



Realizations and mean branch



Mean bifurcation diagram

→ Mean branch $\bar{\gamma}_1$ can be constructed by taking the first coefficient.

Outline

Summary & Outlook

- Bifurcation analysis of the Allen–Cahn equation with random coefficients
  - Turn the stochastic problem into a set of deterministic ones
  - Apply the tools from deterministic bifurcation analysis

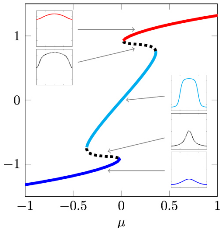
[6] R. Bastiaansen, H. A Dijkstra, and A. S von der Heydt. "Fragmented tipping in a spatially heterogeneous world". In: *Environmental Research Letters* (2022)

Summary & Outlook

❖ Bifurcation analysis of the Allen–Cahn equation with random coefficients

- Turn the stochastic problem into a set of deterministic ones
- Apply the tools from deterministic bifurcation analysis

→ Examine other type of bifurcations, e.g. fold points



$$\partial_t u = \partial_x^2 u + u(1-u^2) + g(x) + \mu^6.$$

[6] R. Bastiaansen, H. A Dijkstra, and A. S von der Heydt. “Fragmented tipping in a spatially heterogeneous world”. In: *Environmental Research Letters* (2022)

Summary & Outlook

- Forward UQ analysis of bifurcations by means of the PC expansion
  - Representation of bifurcation points and branches of equilibria

  → Explore possible structures in the solution, e.g. patterns, travelling waves?

Summary & Outlook

- Forward UQ analysis of bifurcations by means of the PC expansion
  - Representation of bifurcation points and branches of equilibria
  - → Explore possible structures in the solution, e.g. patterns, travelling waves?
- Mean value of the random coefficient is a bifurcation parameter
  - → What about other hyper-parameters of the random field model?

Reference

C. Kuehn, C. Piazzola, and E. Ullmann. “Uncertainty quantification analysis of bifurcations of the Allen–Cahn equation with random coefficients”. In: *Physica D: Nonlinear Phenomena* (2024)

Thank you for the attention!

UNTERSTÜTZT VON / SUPPORTED BY

Alexander von HUMBOLDT STIFTUNG