Computing multiple solutions of partial differential equations

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Section 1

Introduction

Can you conduct an experiment twice . . .

and get two different answers?

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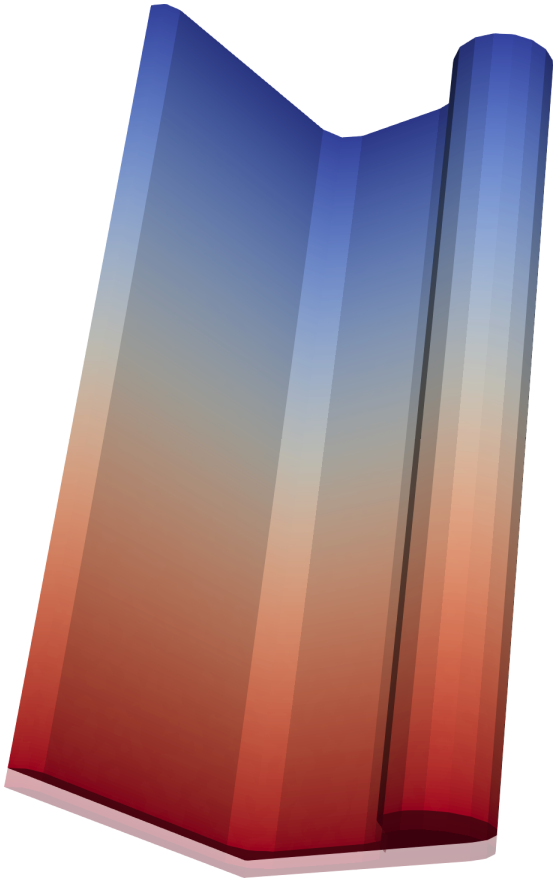

Axial displacement test of an Embraer aircraft stiffener.

Can you conduct an experiment twice . . .

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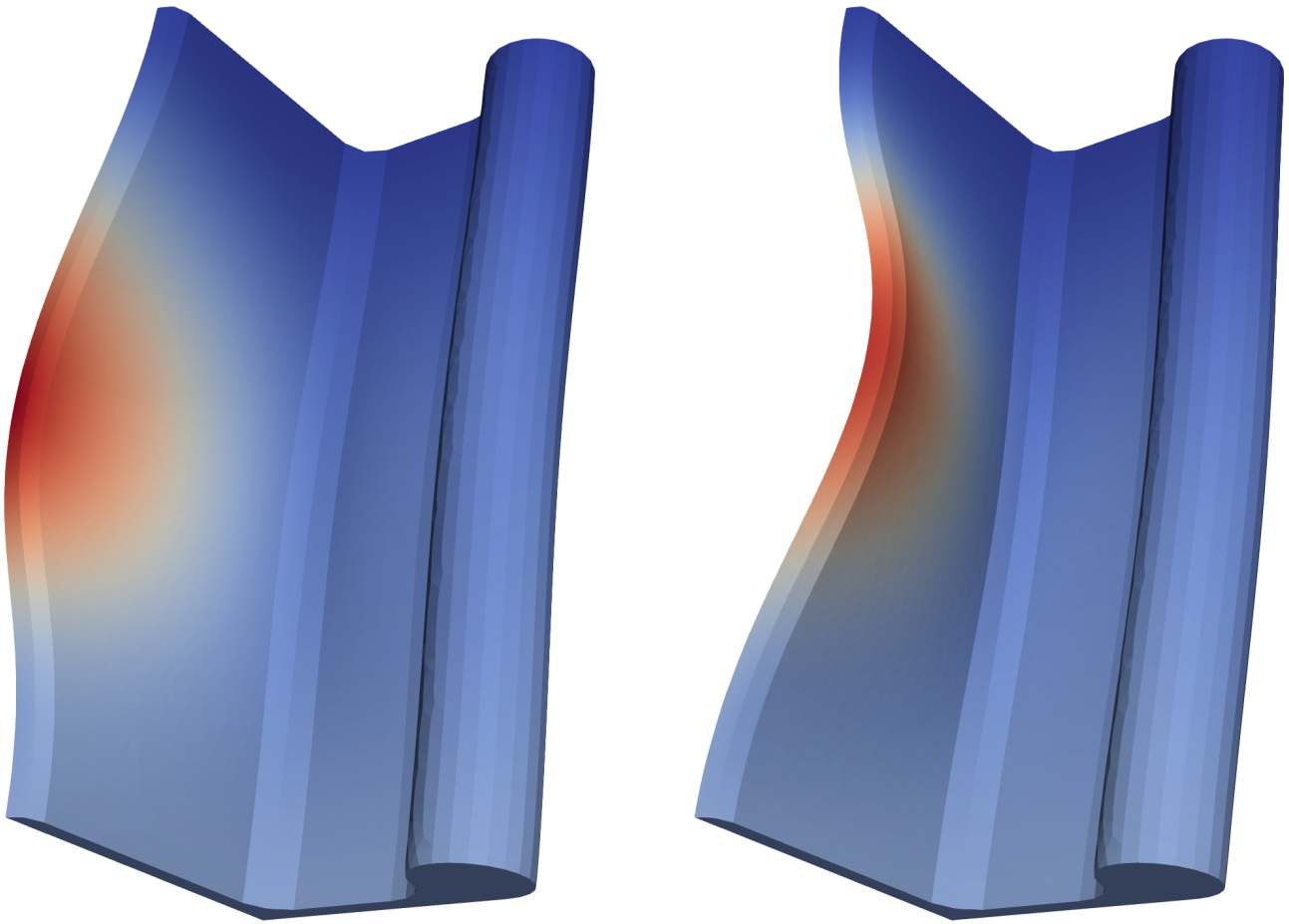

Two different, stable configurations.

Mathematical formulation

Compute the multiple *solutions* u of an equation

$$f(u, \lambda) = 0$$
$$f : V \times \mathbb{R} \to V^*$$

as a function of a parameter λ.

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u displacement, λ loading, f hyperelasticity

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Aircraft stiffener

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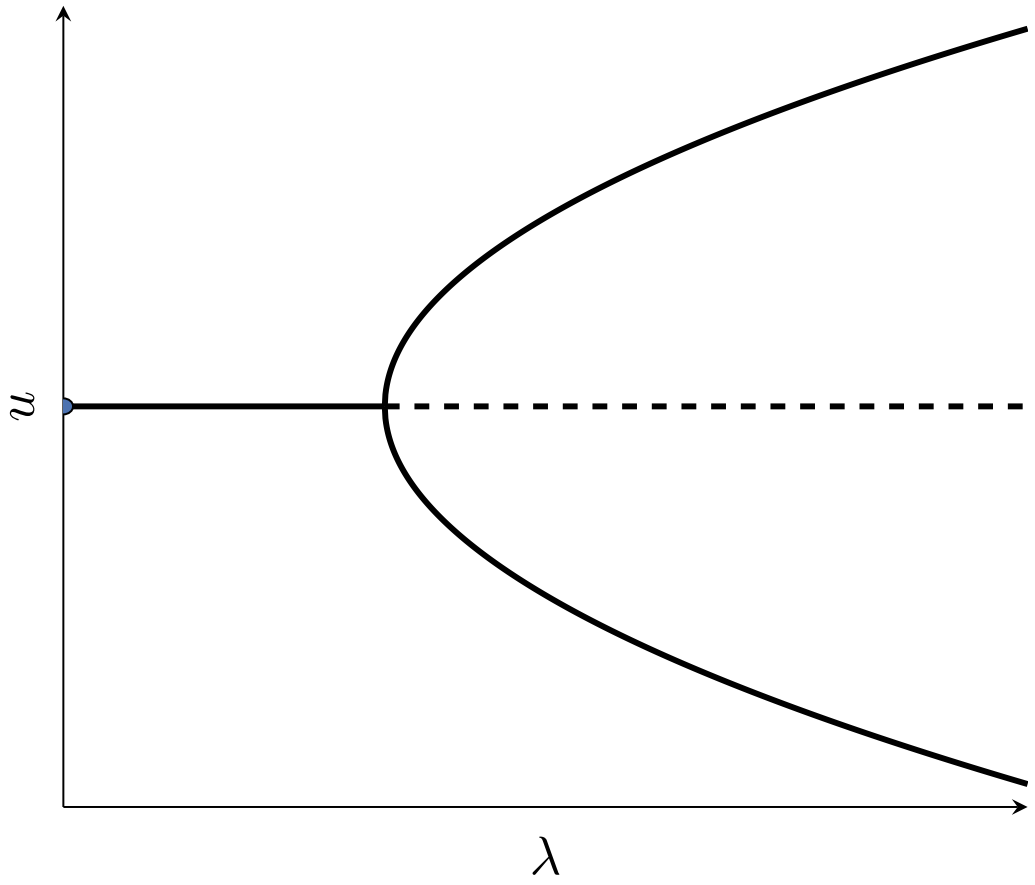
Today

u director field or Q-tensor, f Oseen–Frank or Landau–de Gennes

Section 2

The classical algorithm

Branch switching



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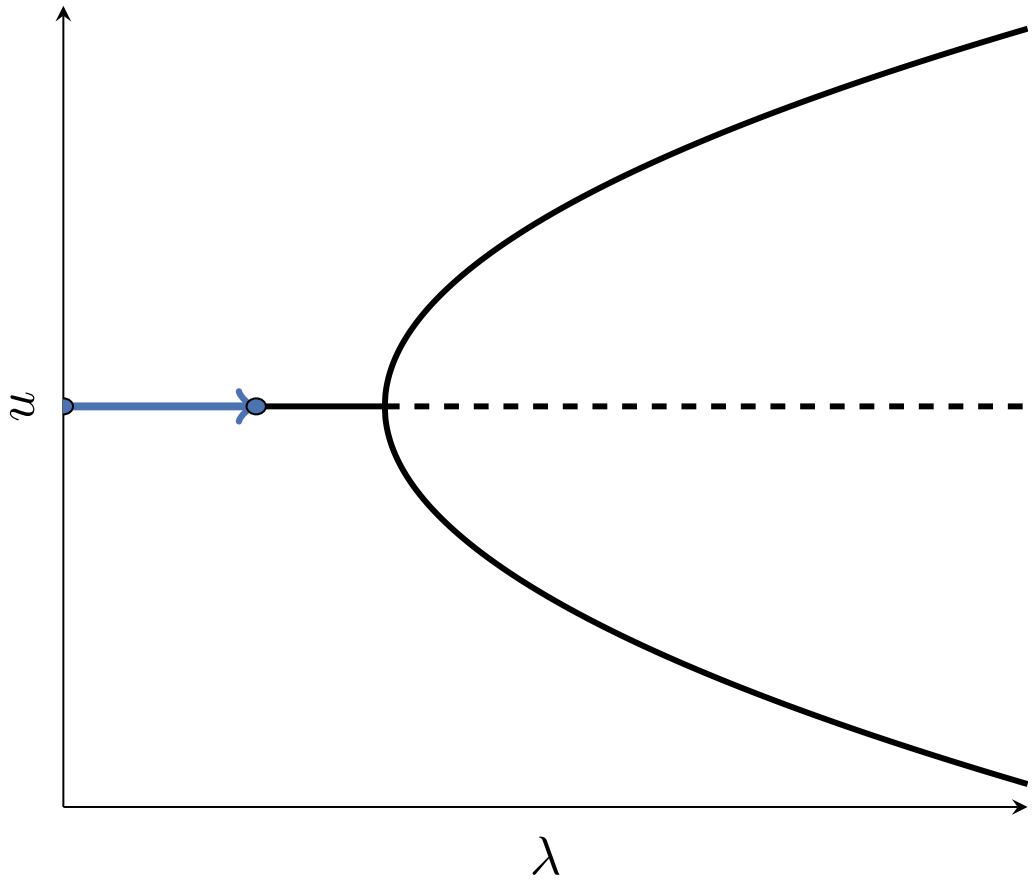
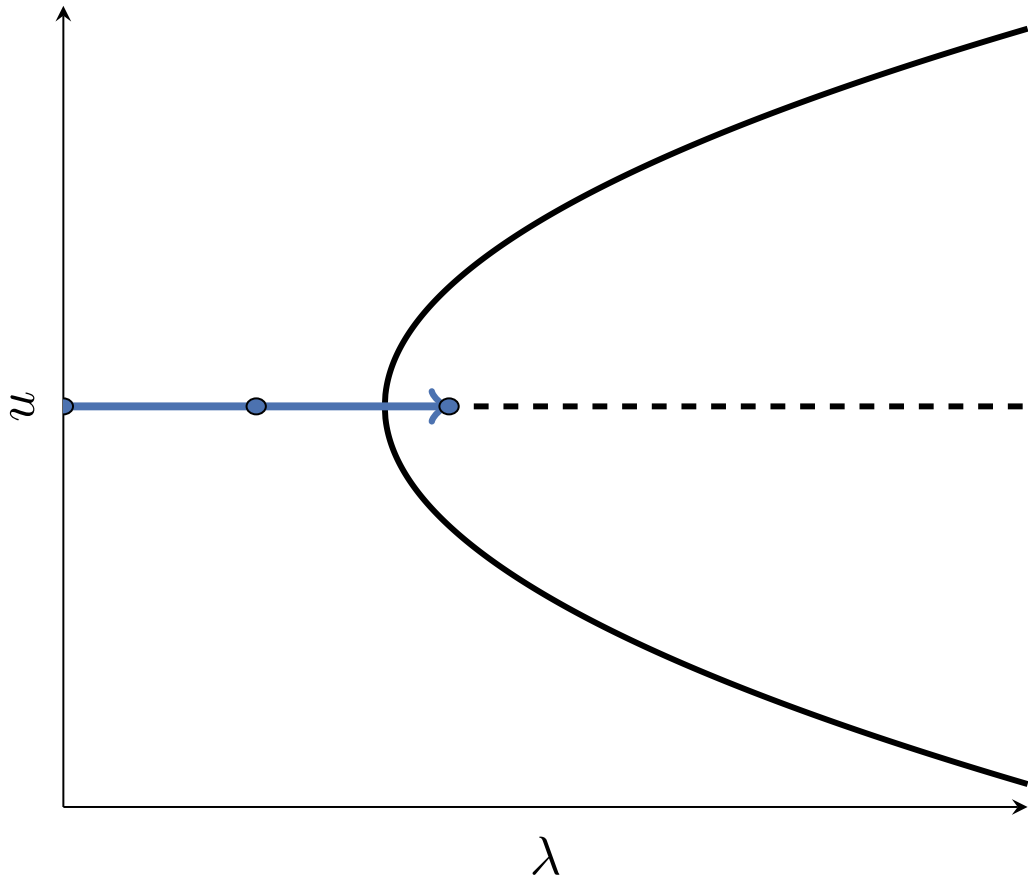


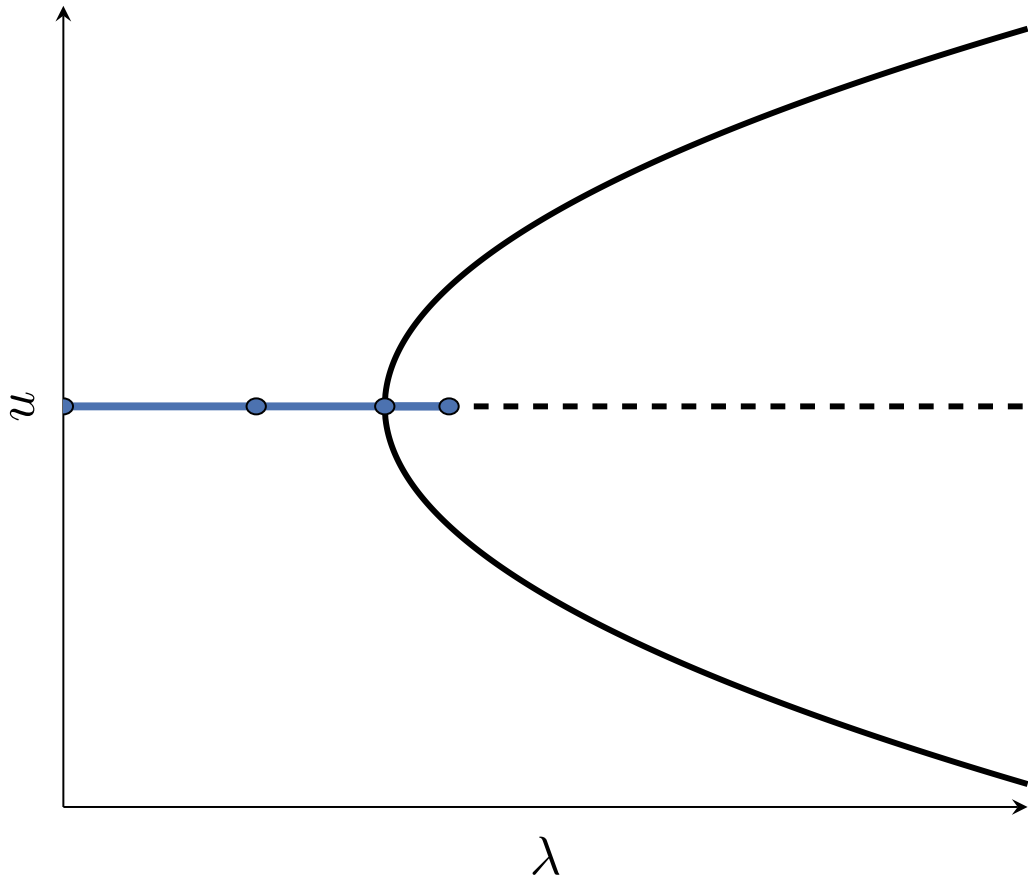
Step I: continuation

Branch switching



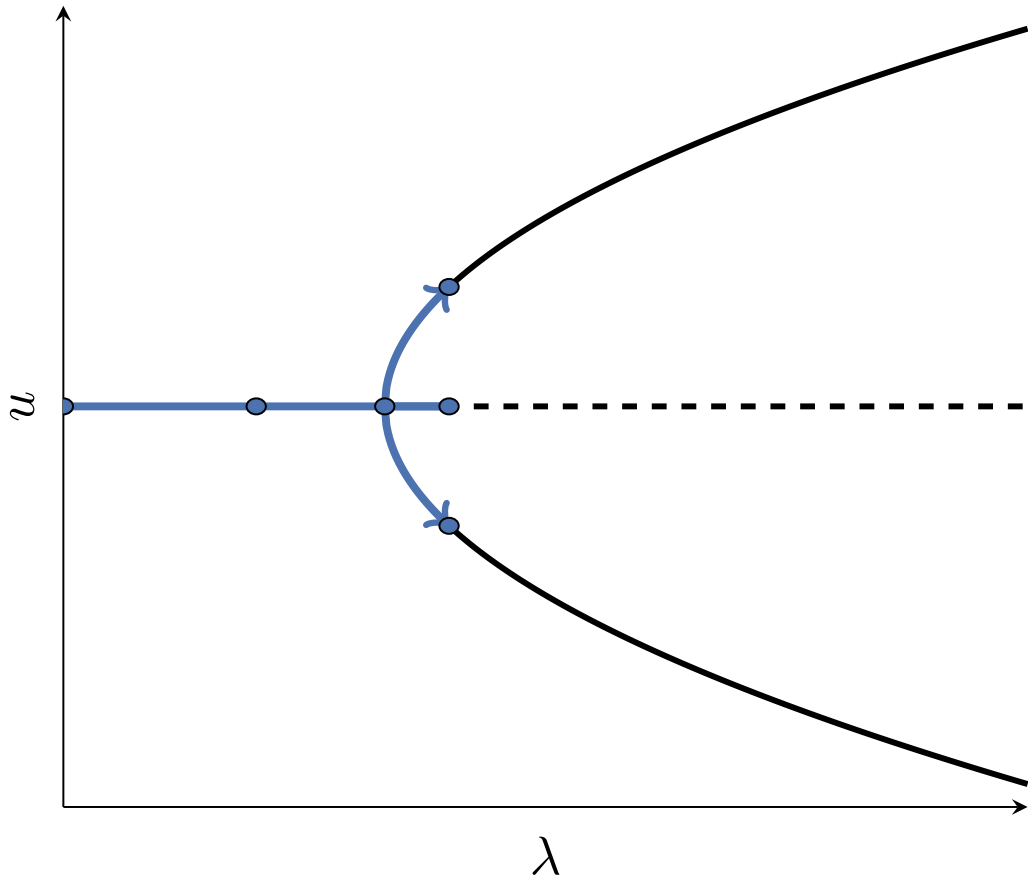
Step II: continuation

Branch switching



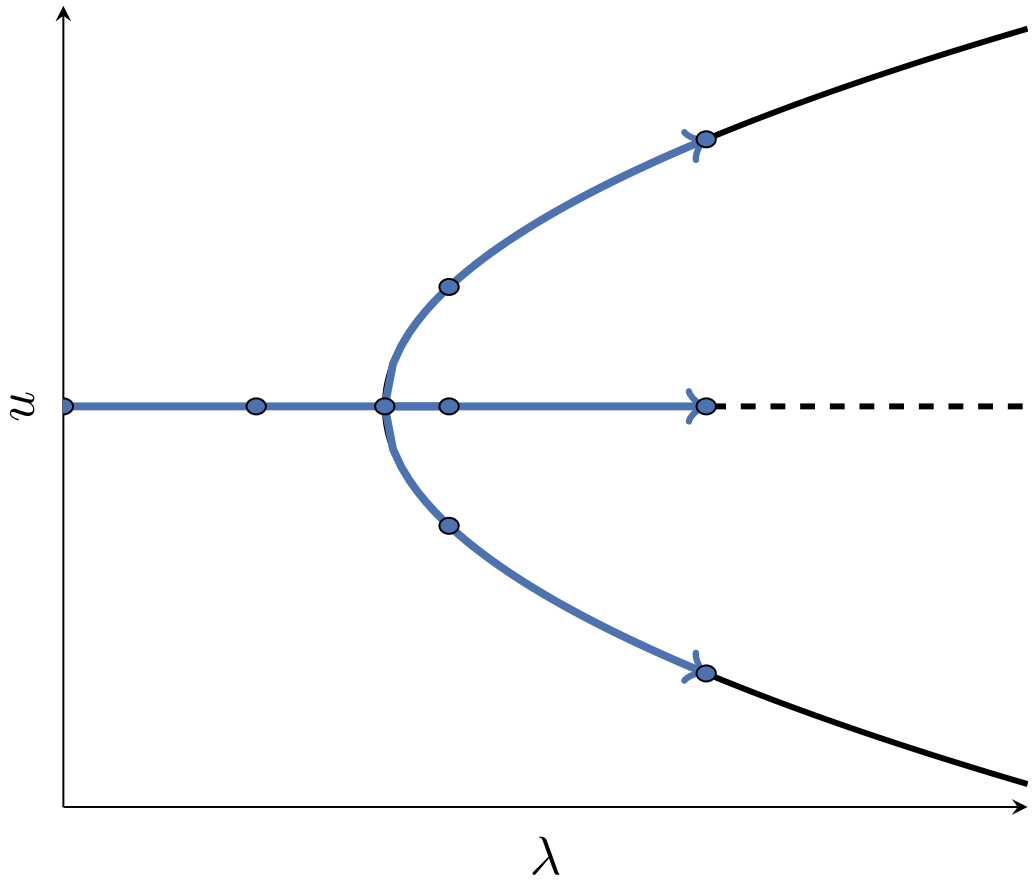
Step III: detect bifurcation point

Branch switching



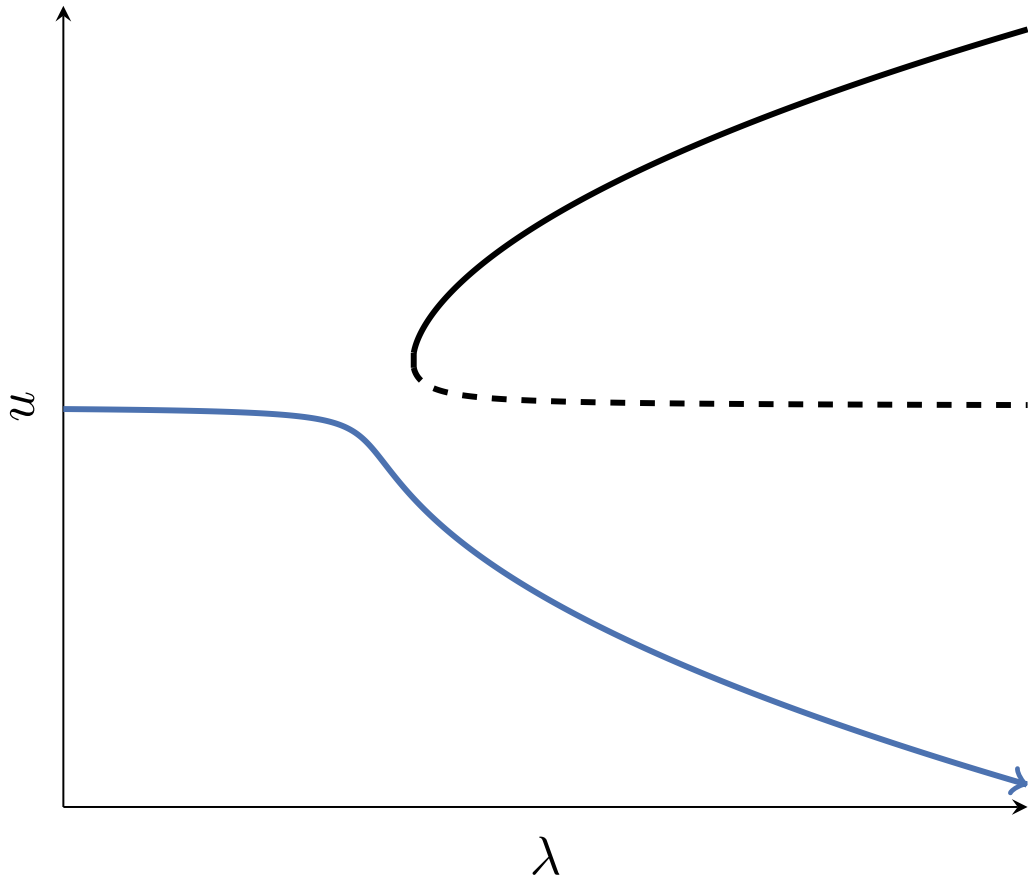
Step IV: compute eigenvectors and switch

Branch switching



Step V: continuation on branches

Branch switching



A disconnected diagram.

Branch switching

Disconnected diagrams

The algorithm only computes branches connected to the initial datum.

This work

Disconnected diagrams

An algorithm that can compute **disconnected bifurcation diagrams**.

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Disconnected diagrams

An algorithm that can compute **disconnected bifurcation diagrams**.

Scaling

The computational kernel is exactly the same as Newton's method.

Section 3

Deflation

The core idea

Deflation

Fix parameter λ. Given

- a Fréchet differentiable residual $\mathcal{F} : V \to V^*$
- a solution $r \in V$, $\mathcal{F}(r) = 0$, $\mathcal{F}'(r)$ nonsingular

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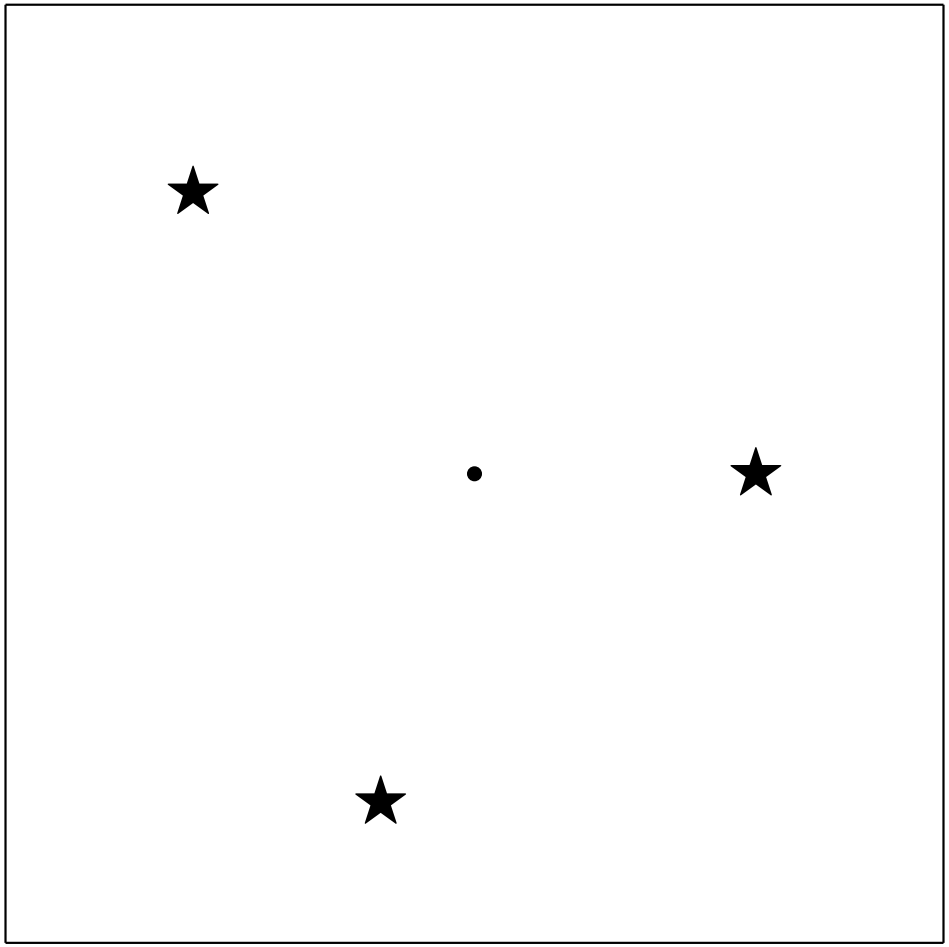
Find more solutions, starting from the same initial guess.

Finding many solutions from the same guess



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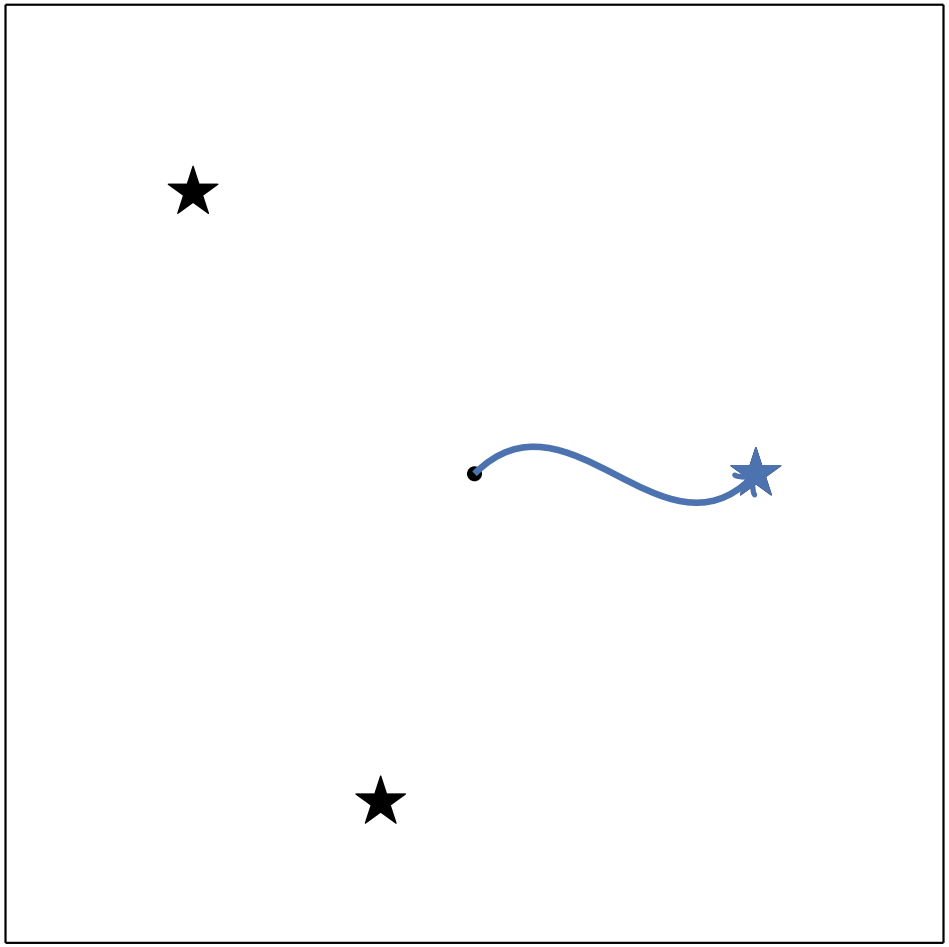
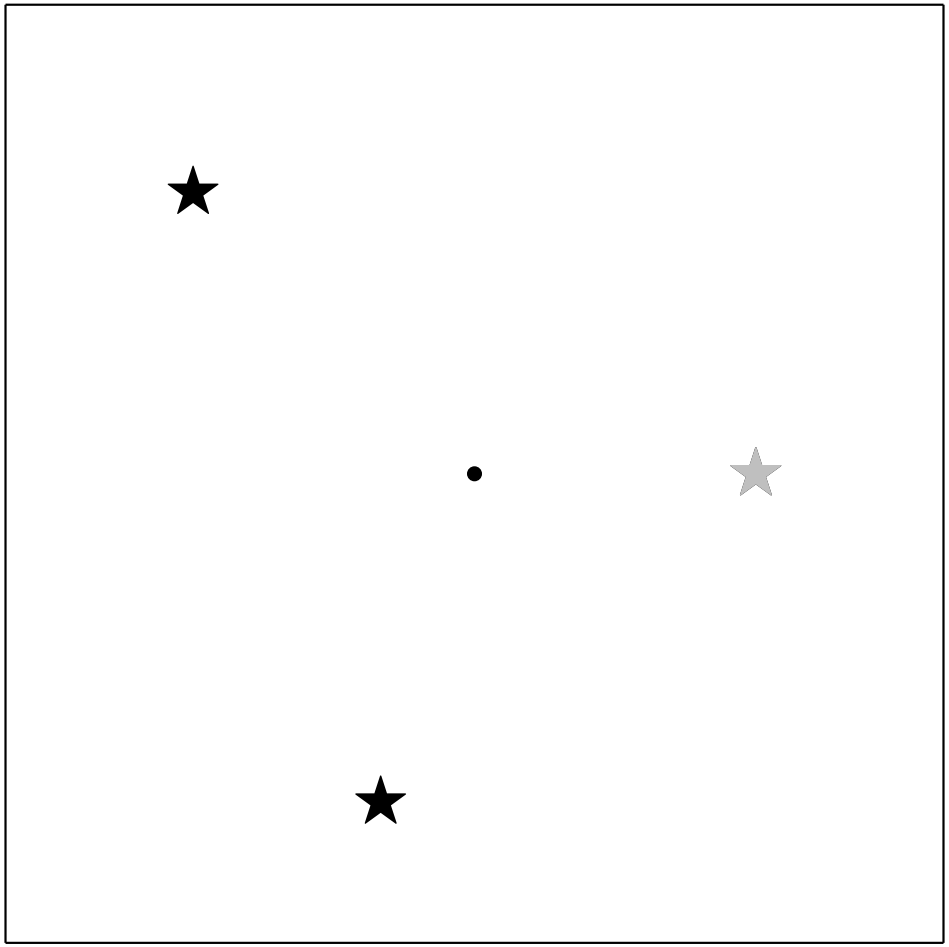


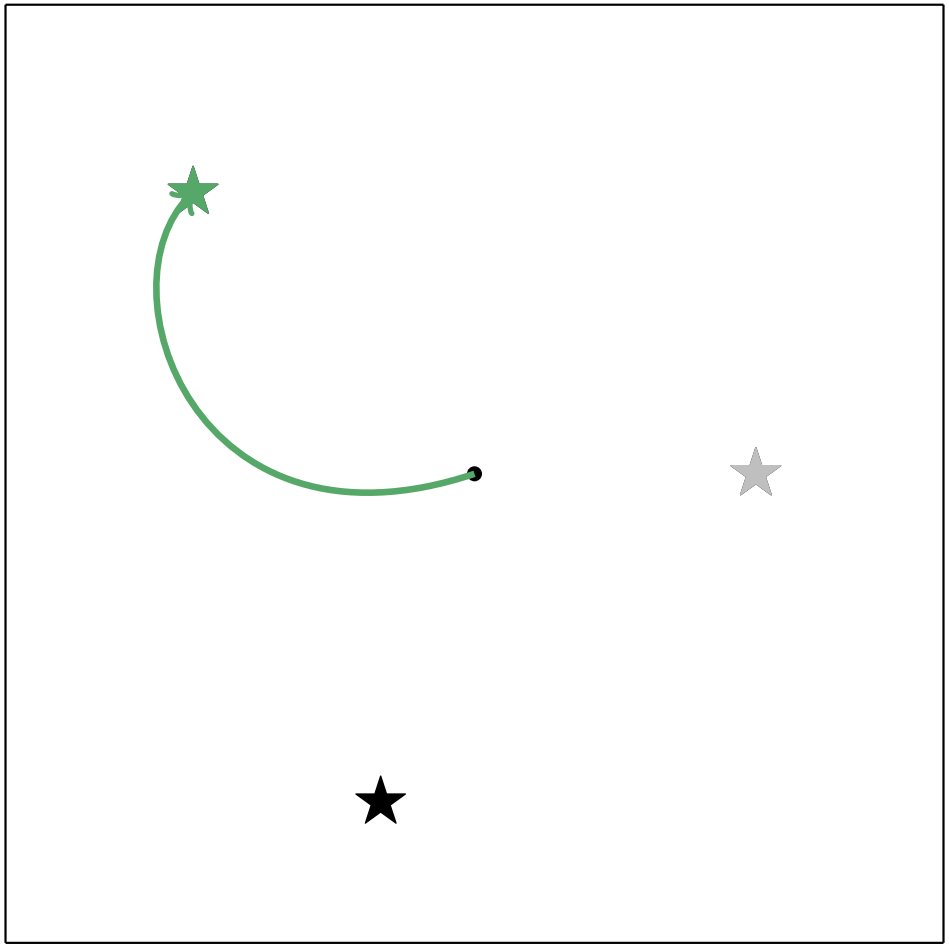
Step I: Newton from initial guess

Finding many solutions from the same guess



Step II: deflate solution found

Finding many solutions from the same guess



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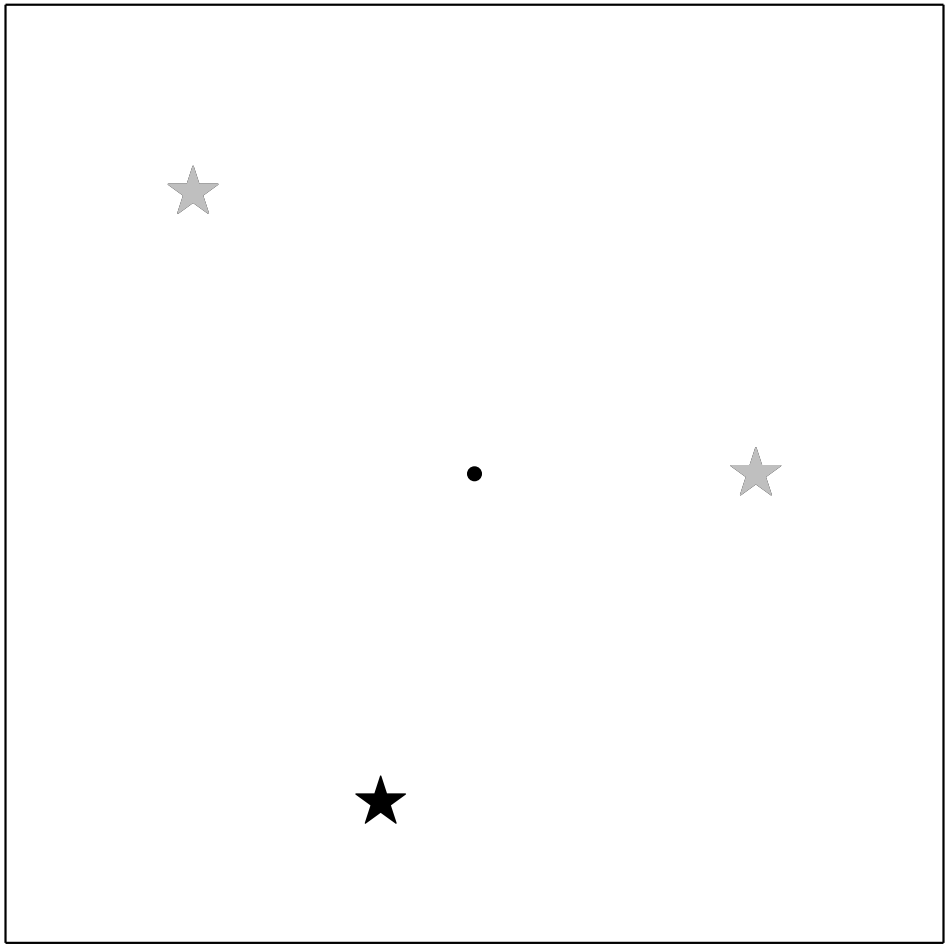

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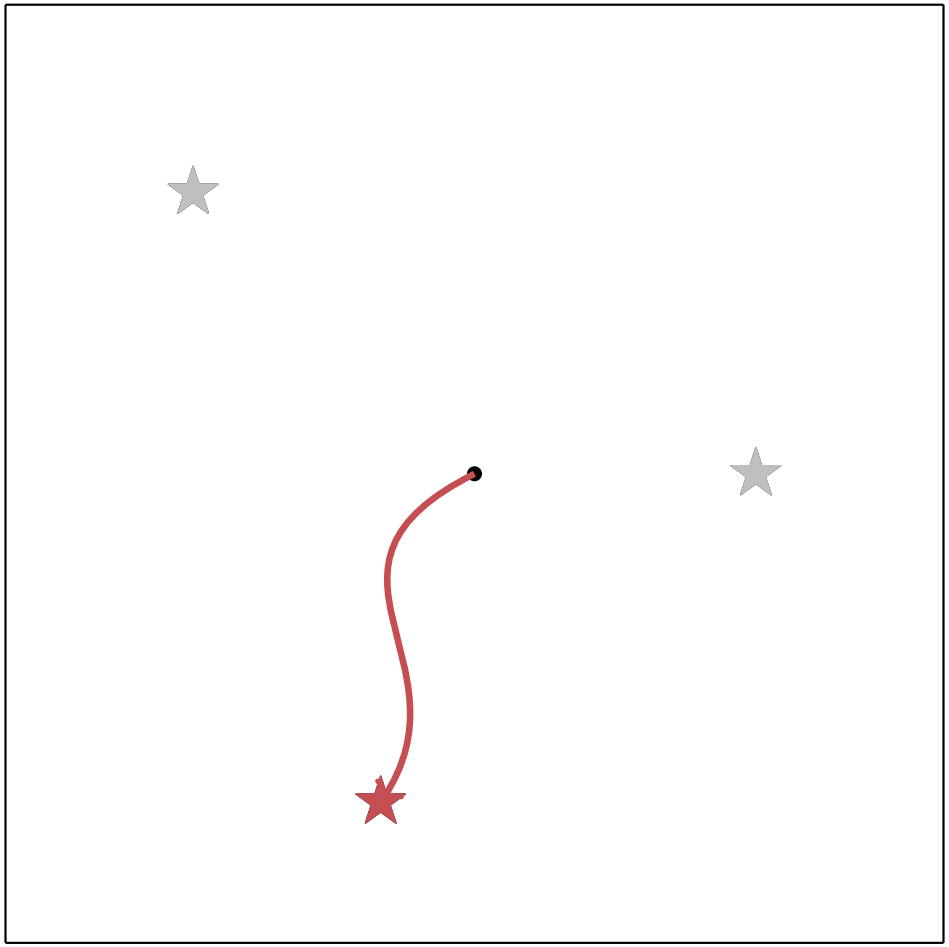

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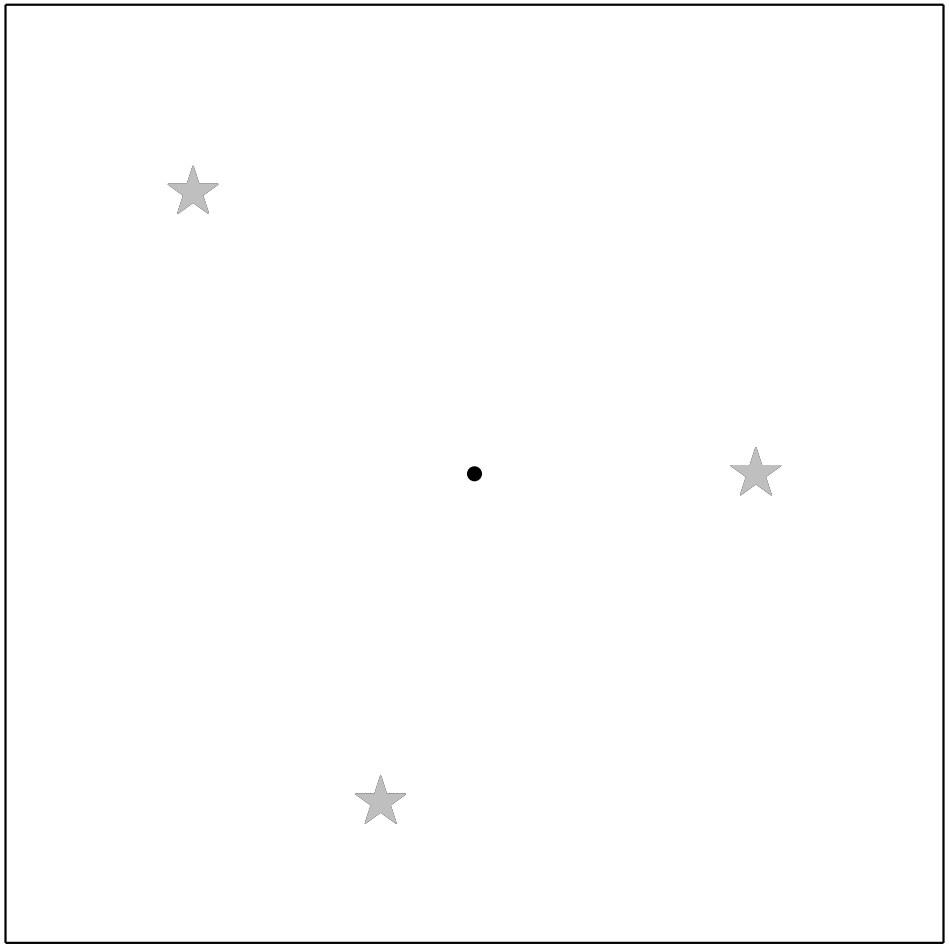

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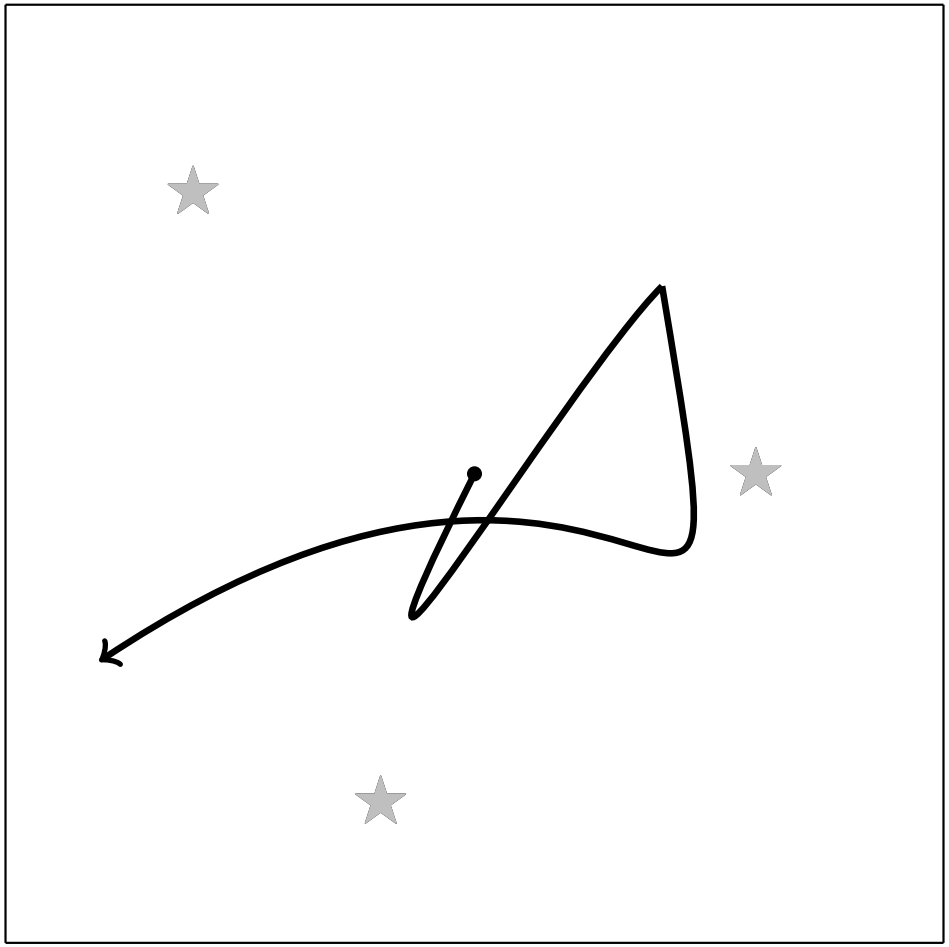

Step III: termination on nonconvergence

Finding many solutions from the same guess

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Construction of deflated problems

A nonlinear transformation

$$\mathcal{G}(u) = \mathcal{M}(u; r)\mathcal{F}(u)$$

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A deflation operator

We say $\mathcal{M}(u; r)$ is a deflation operator if for any sequence $u \to r$

$$\liminf_{u \to r} \|\mathcal{G}(u)\|_{V^*} = \liminf_{u \to r} \|\mathcal{M}(u; r)\mathcal{F}(u)\|_{V^*} > 0$$

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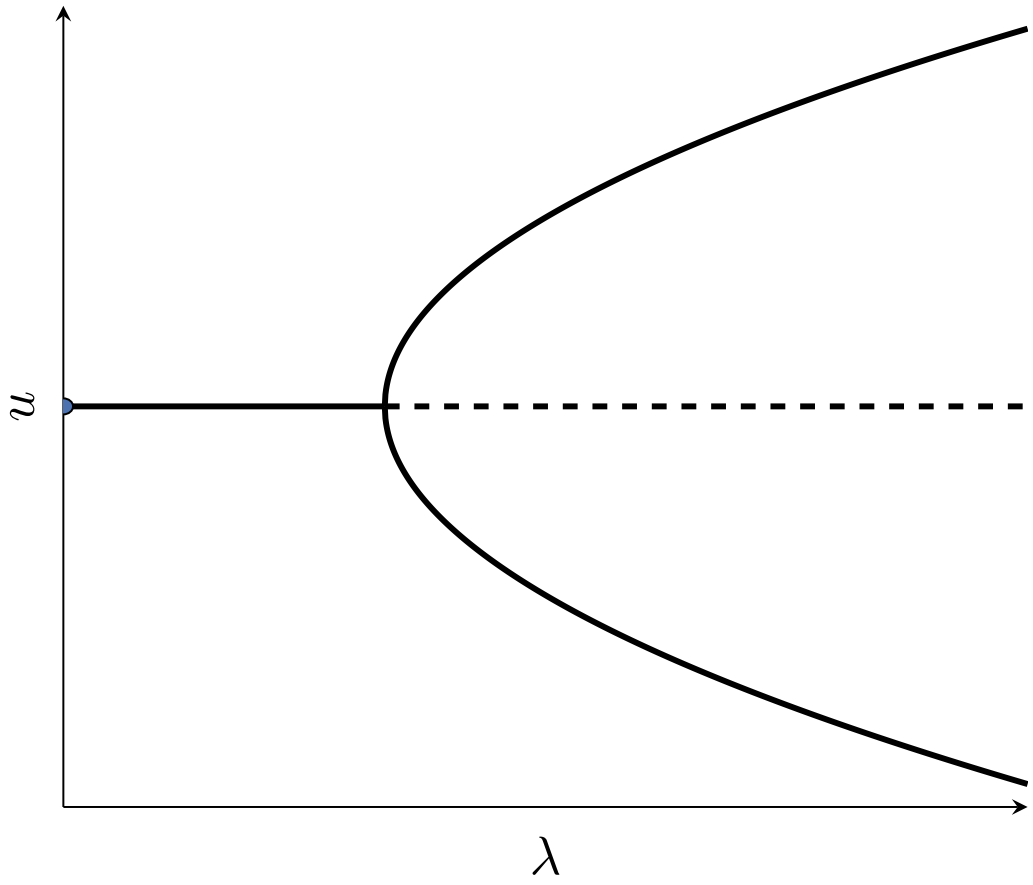
Theorem (F., Birkisson, Funke, 2014)

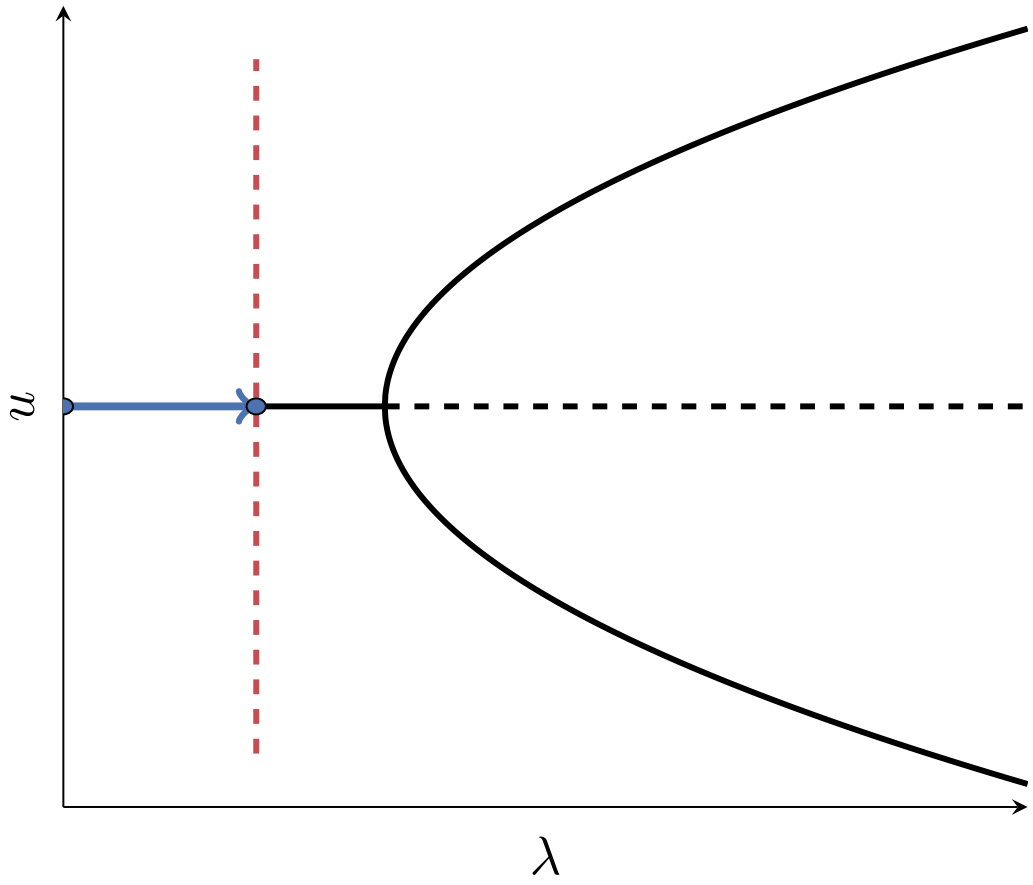
This is a deflation operator for $p \geq 1$:

$$\mathcal{M}(u; r) = \left(\frac{1}{\|u - r\|^p} + 1 \right)$$

Deflated continuation

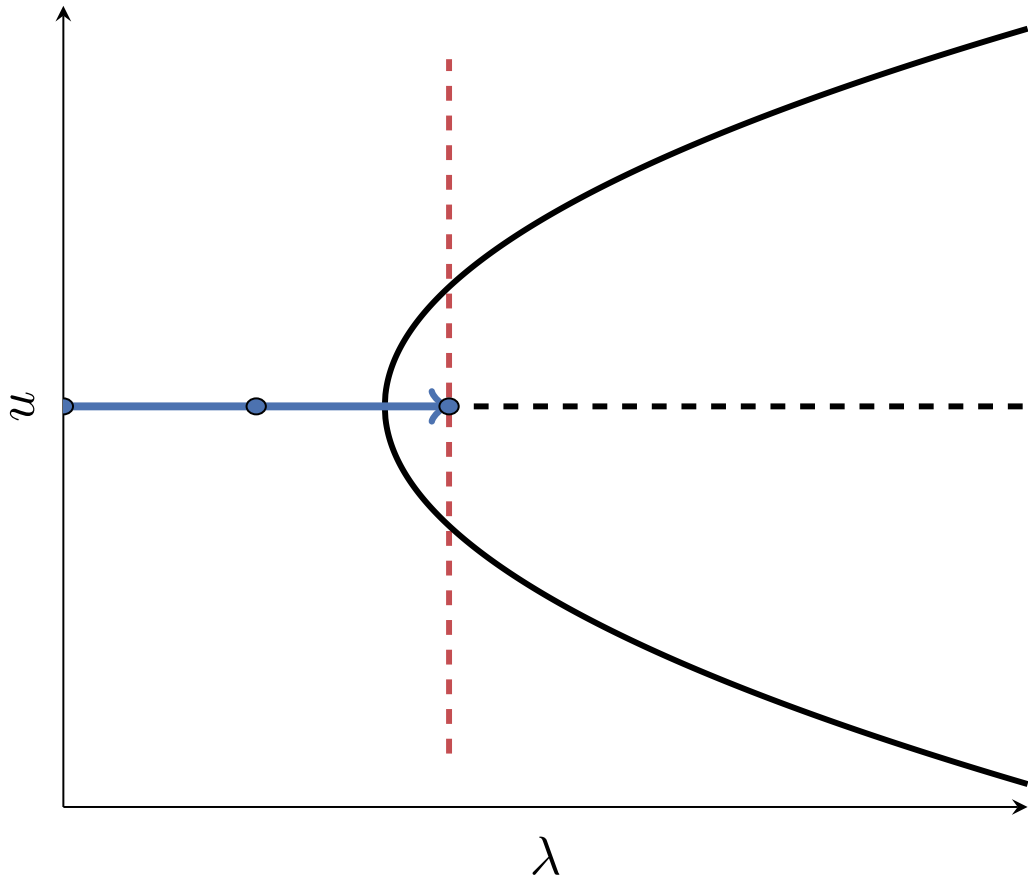


Deflated continuation



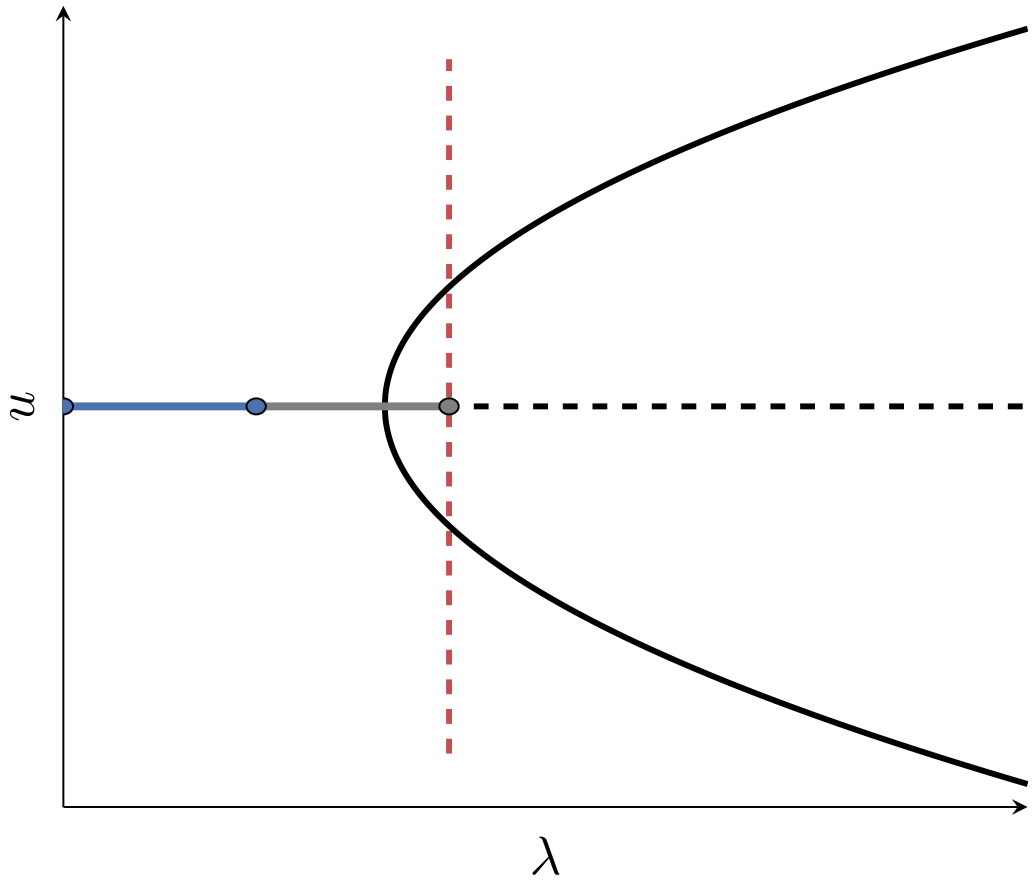
Step I: continuation

Deflated continuation



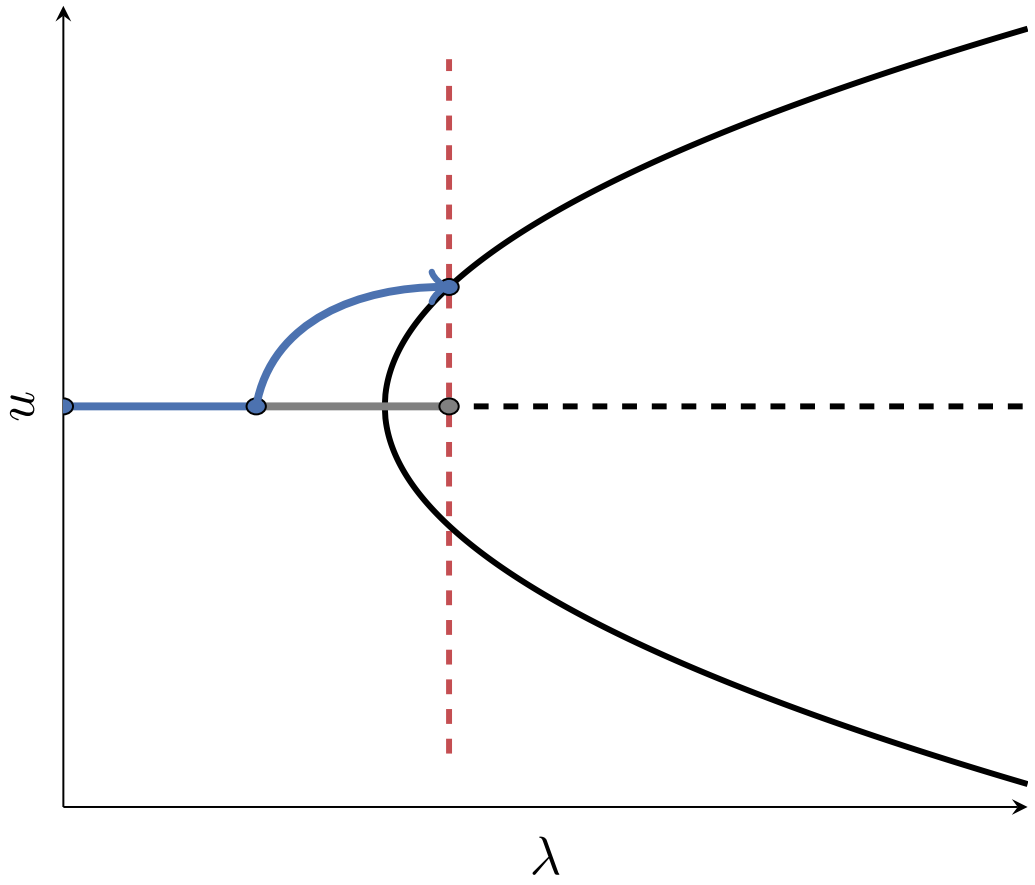
Step II: continuation

Deflated continuation



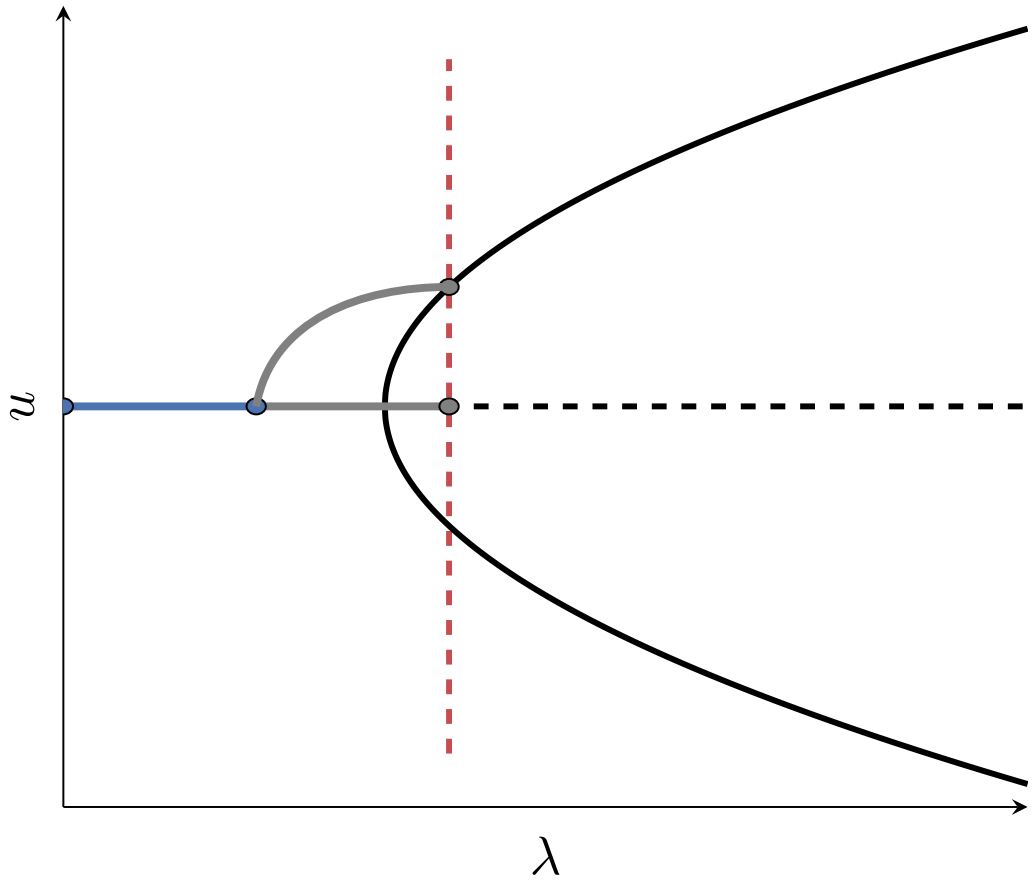
Step III: deflate

Deflated continuation



Step III+: solve deflated problem

Deflated continuation



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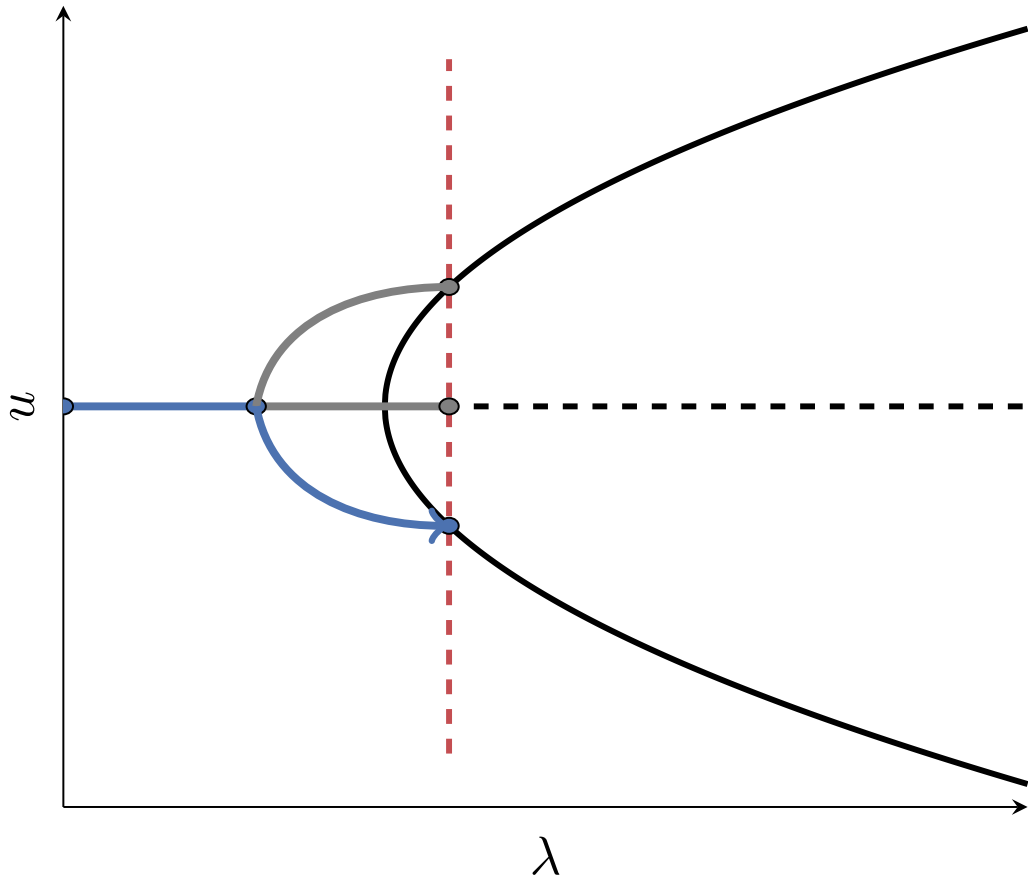
Deflated continuation



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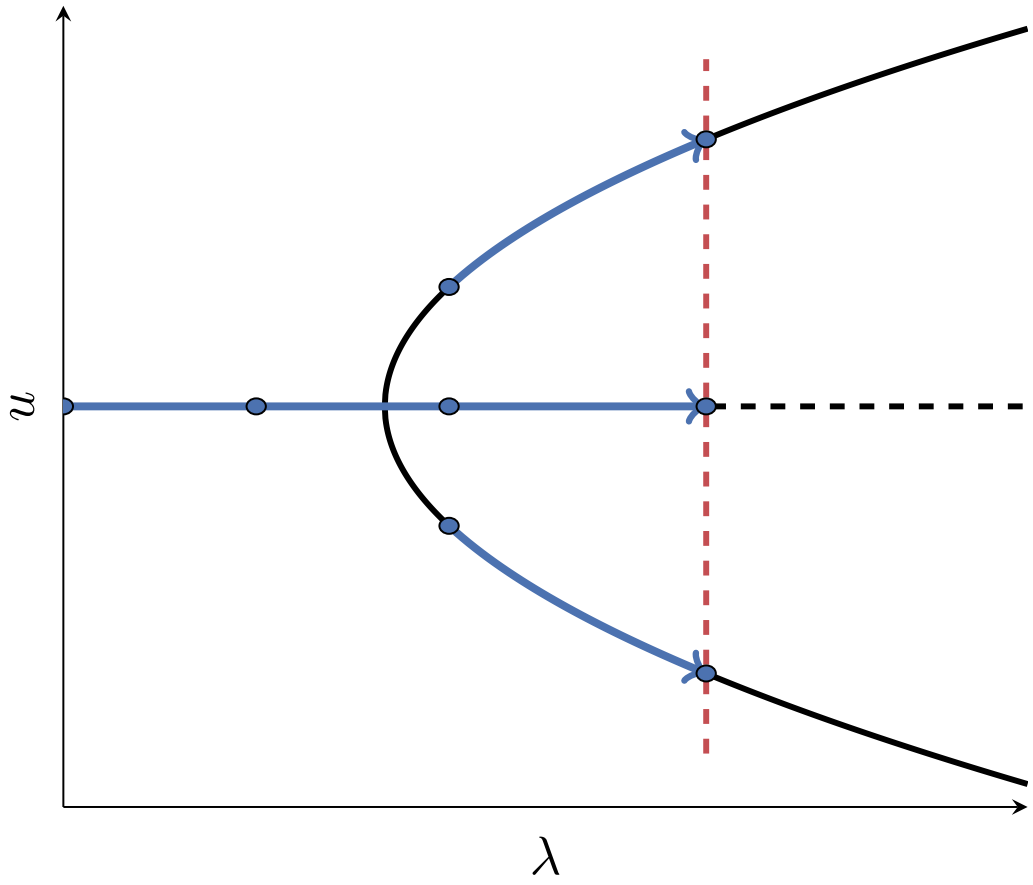
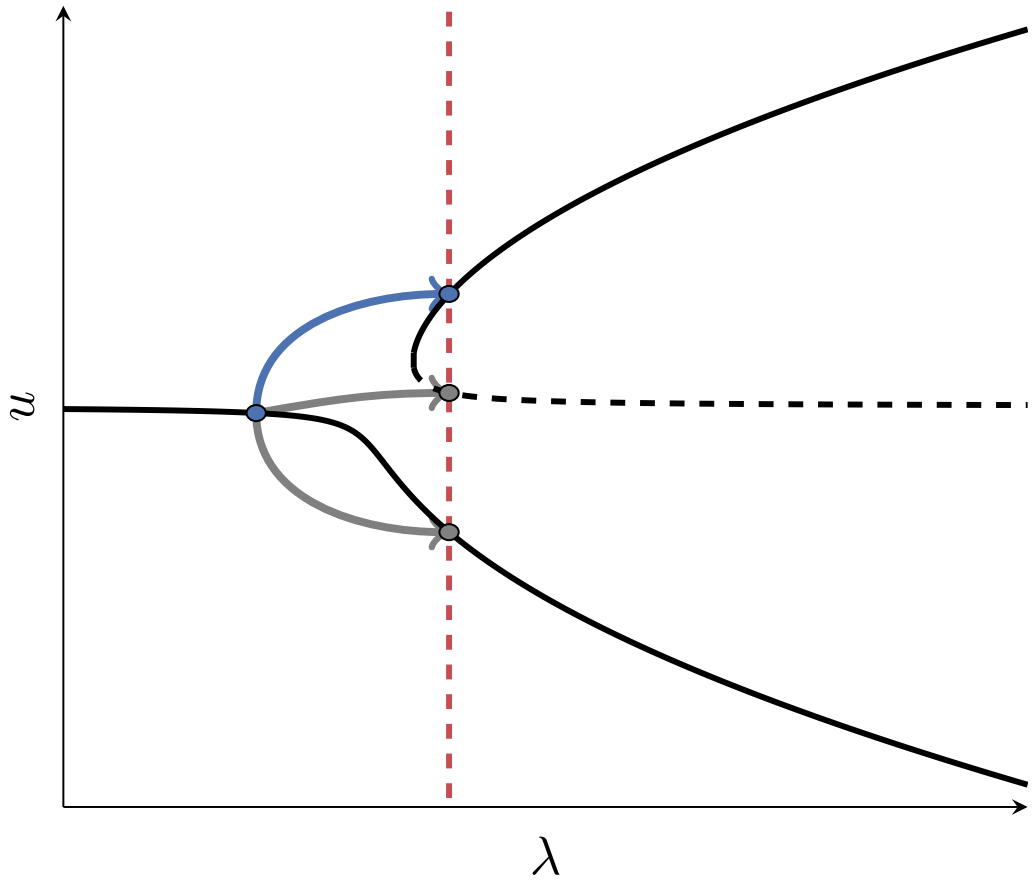


Step IV: continuation on branches

Deflated continuation



A disconnected diagram.

Section 4

Computations

Newton–Krylov

A question

How do we solve the deflated problem?

Newton–Krylov

A Newton step

$$J_F(u)\Delta u_F = -F(u)$$

Newton–Krylov

A Newton step

$$J_F(u)\Delta u_F = -F(u)$$

A deflated Newton step

$$J_G(u)\Delta u_G = -G(u)$$

Newton–Krylov

A Newton step

$$J_F(u)\Delta u_F = -F(u)$$

A deflated Newton step

$$J_G(u)\Delta u_G = -G(u)$$

Deflated residual

$$G(u) = M(u;r)F(u)$$

Newton–Krylov

A Newton step

$$J_F(u)\Delta u_F = -F(u)$$

A deflated Newton step

$$J_G(u)\Delta u_G = -G(u)$$

Deflated Jacobian

$$J_G(u) = M(u;r)J_F(u) + F(u)M'(u;r)^T$$

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Newton–Krylov

A Newton step

$$J_F(u)\Delta u_F = -F(u)$$

A deflated Newton step

$$J_G(u)\Delta u_G = -G(u)$$

Sherman–Morrison–Woodbury

$$\Delta u_G = \tau \Delta u_F$$

where $\tau \in \mathbb{R}$ is a simple function of $J_F^{-1}F, M$, and M'.

Newton–Krylov

Scaling of deflated continuation

With a good preconditioner, you can do bifurcation analysis at scale.

Section 5

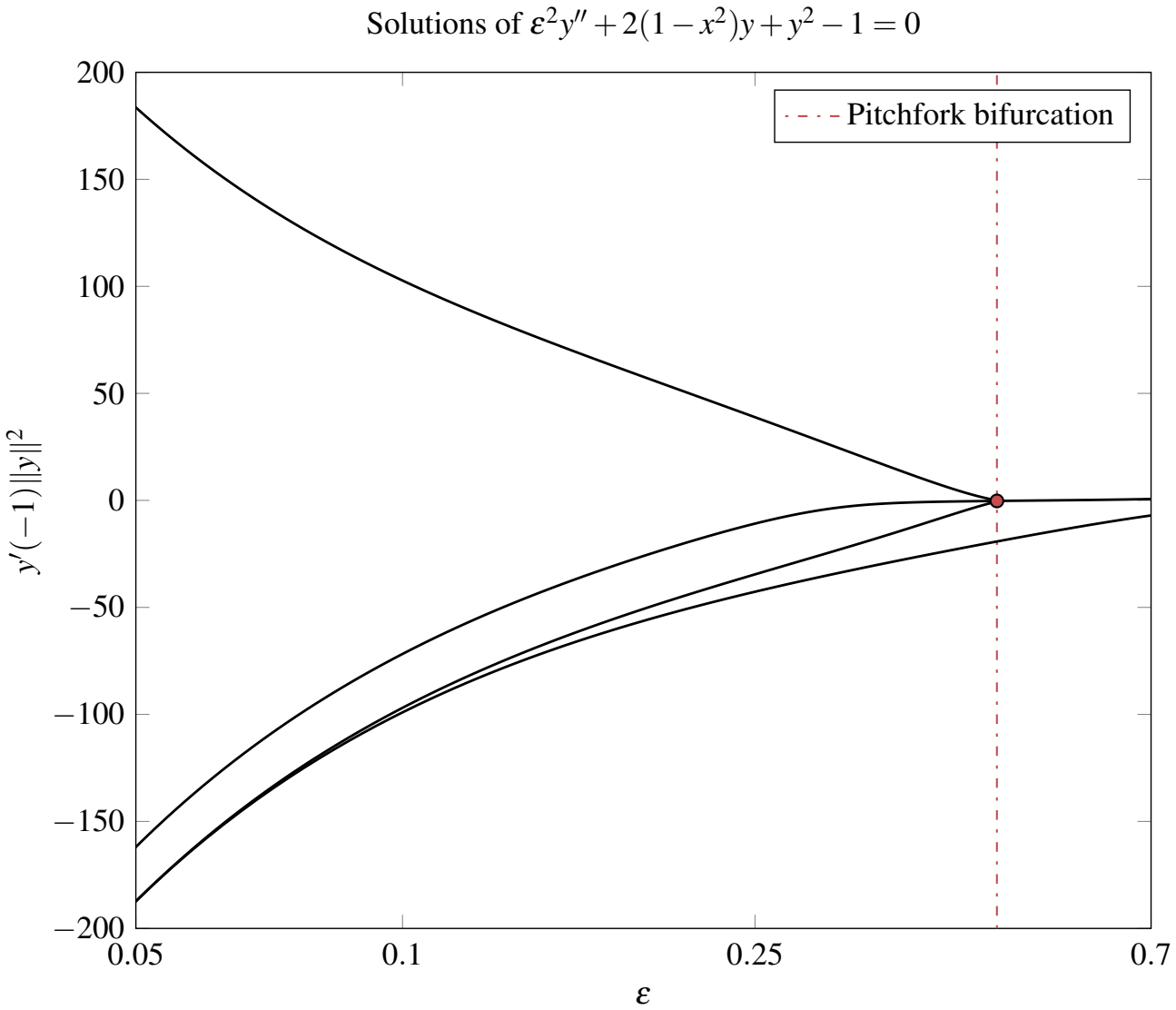
Applications

Application: Carrier's problem

Carrier's problem (Carrier 1970, Bender & Orszag 1999)

$$\varepsilon^2 y'' + 2(1 - x^2)y + y^2 - 1 = 0, \quad y(-1) = 0 = y(1).$$

Application: Carrier's problem



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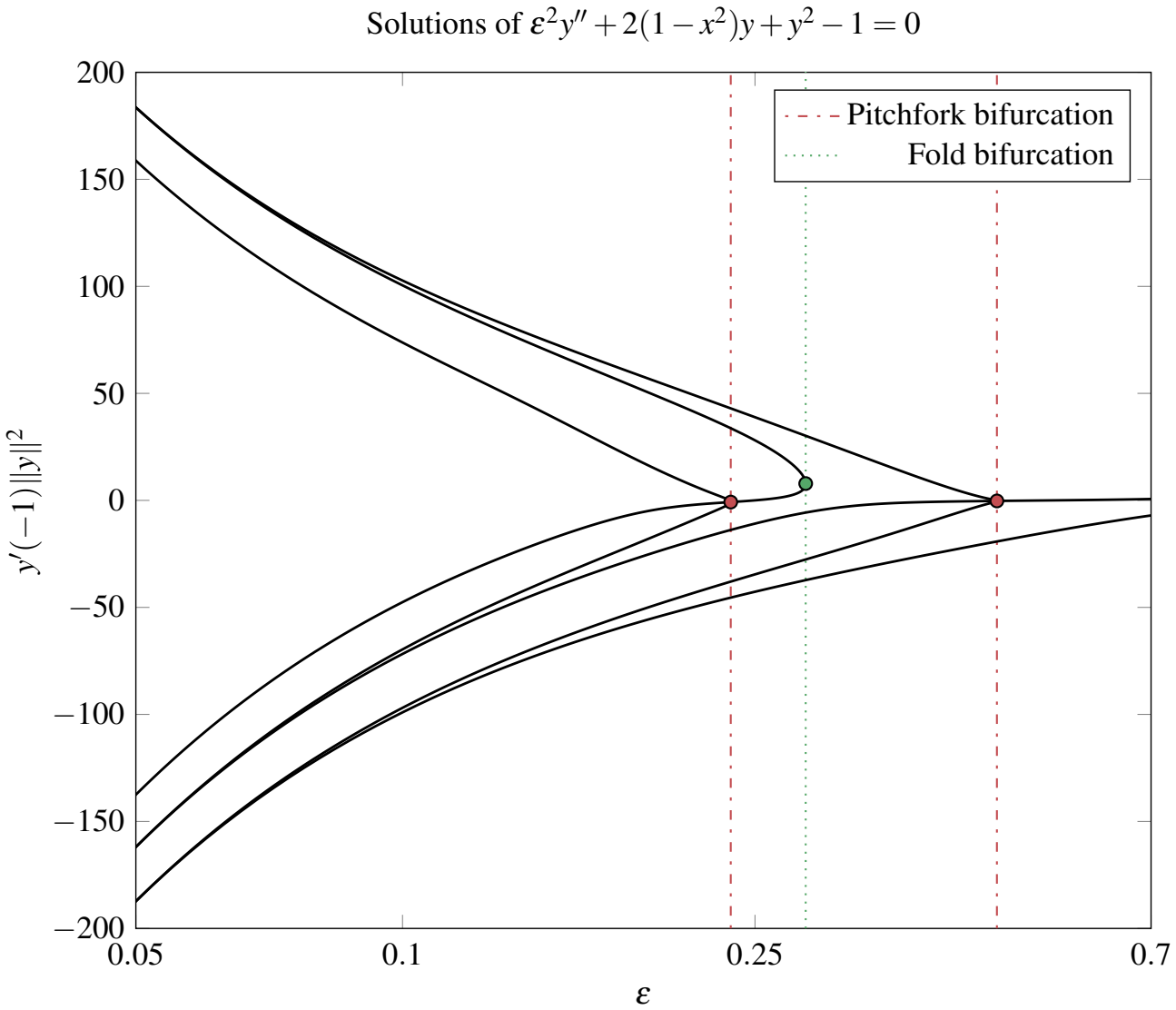

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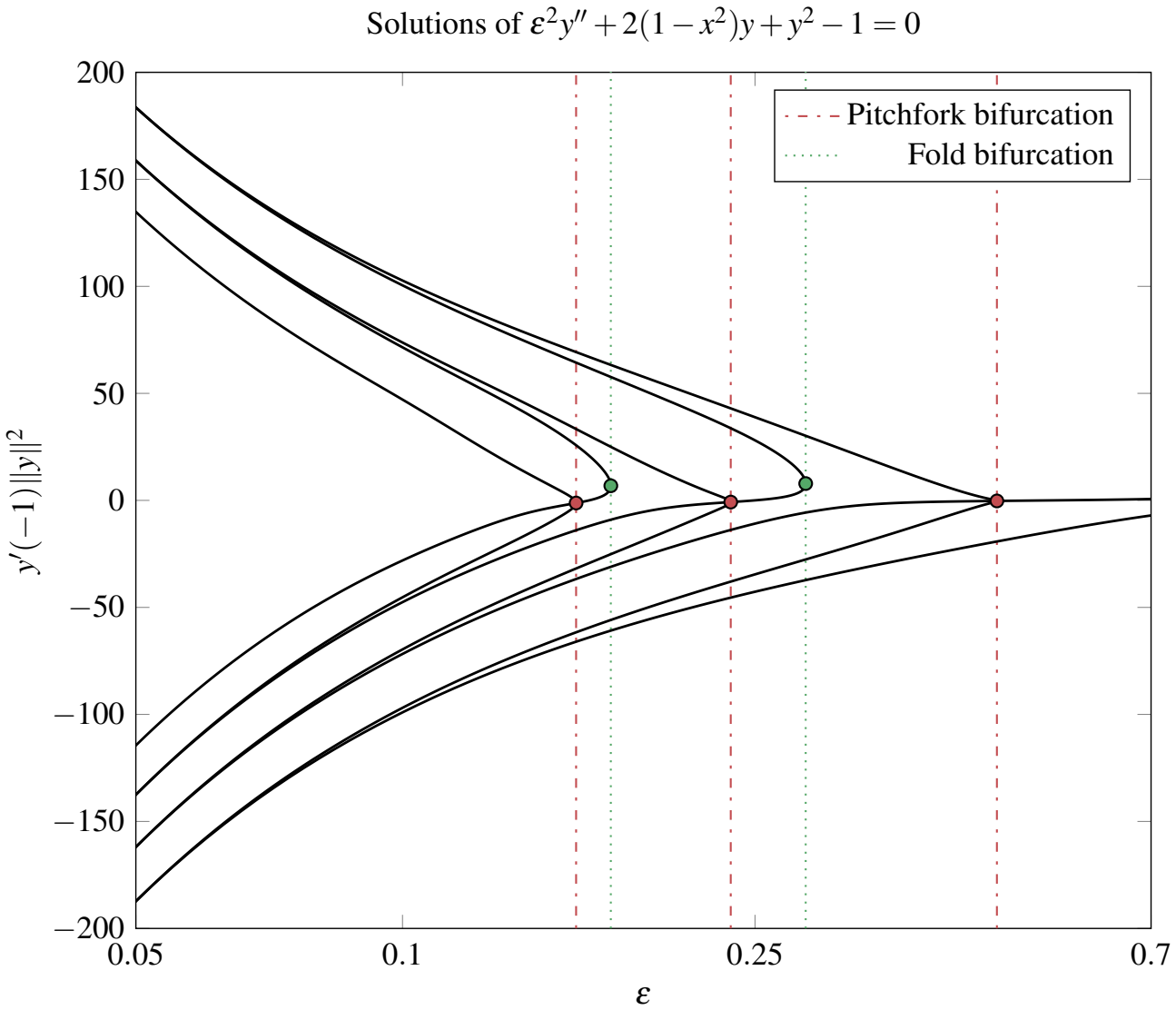

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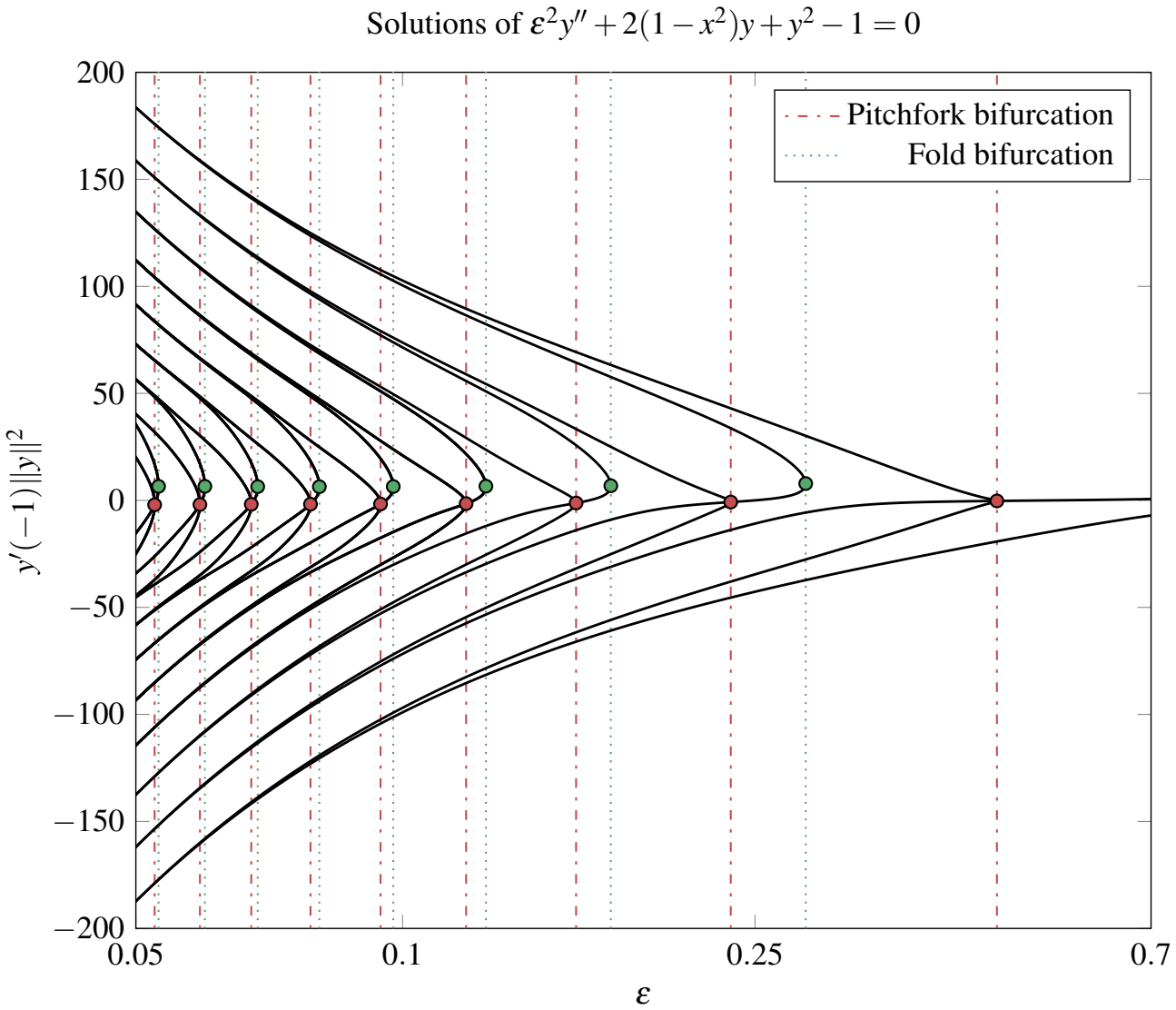


Application: Carrier's problem

Pitchfork bifurcations

$$\varepsilon \approx \frac{0.472537}{n}$$

Application: Carrier's problem

Pitchfork bifurcations

$$\varepsilon \approx \frac{0.472537}{n}$$

Connected component	Computed ε	Asymptotic estimate	Relative error
1	0.46886251	0.472537	0.7837%
2	0.23472529	0.236269	0.6574%
3	0.15703946	0.157512	0.3012%
4	0.11798359	0.118134	0.1278%

Computed and estimated parameter values for the first four pitchfork bifurcations.

Application: Carrier's problem

Fold bifurcations

$$\varepsilon \approx \frac{0.472537}{n - \frac{0.8344}{n}}$$

Application: Carrier's problem

Fold bifurcations

$$\varepsilon \approx \frac{0.472537}{n - \frac{0.8344}{n}}$$

Connected component	Computed ε	Asymptotic estimate	Relative error
2	0.28522538	0.298545	4.670%
3	0.17186970	0.173608	1.011%
4	0.12421206	0.124634	0.3397%
5	0.09762446	0.0977706	0.1497%

Computed and estimated parameter values for the first four fold bifurcations.

Application: Freedericksz transition

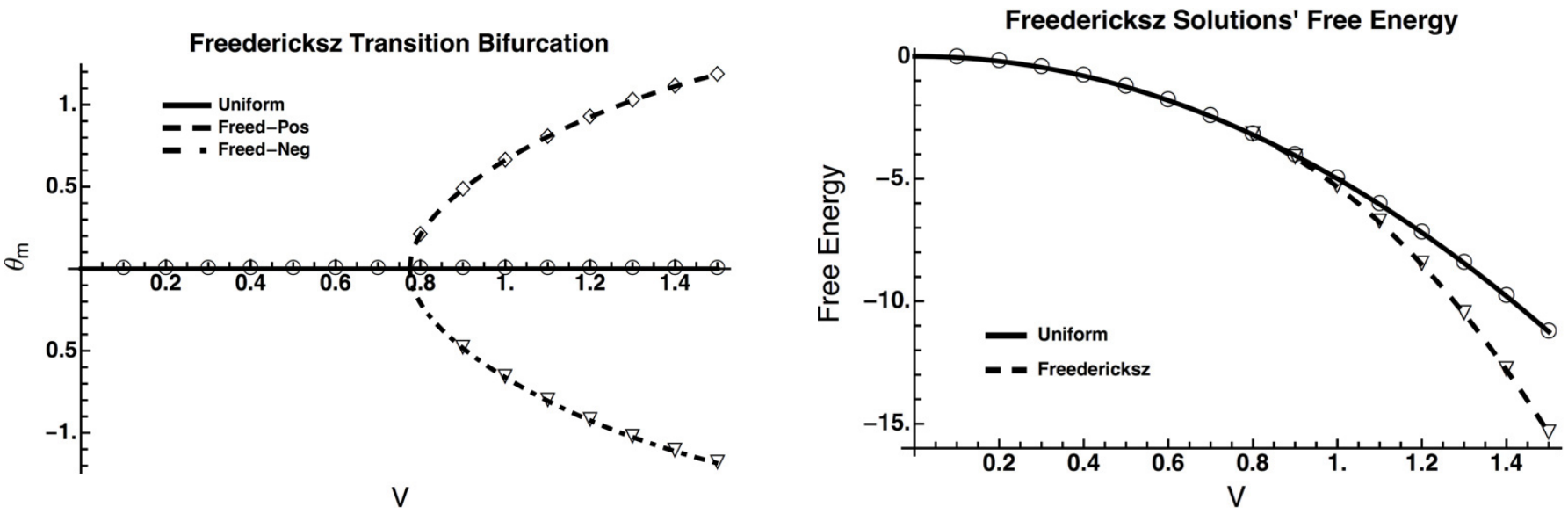
Description

A classical pitchfork bifurcation. Below a certain electric field threshold, the liquid crystal remains undistorted. Beyond a critical strength V, the director twists to align with the field.

Minimise Oseen–Frank energy on a unit square subject to

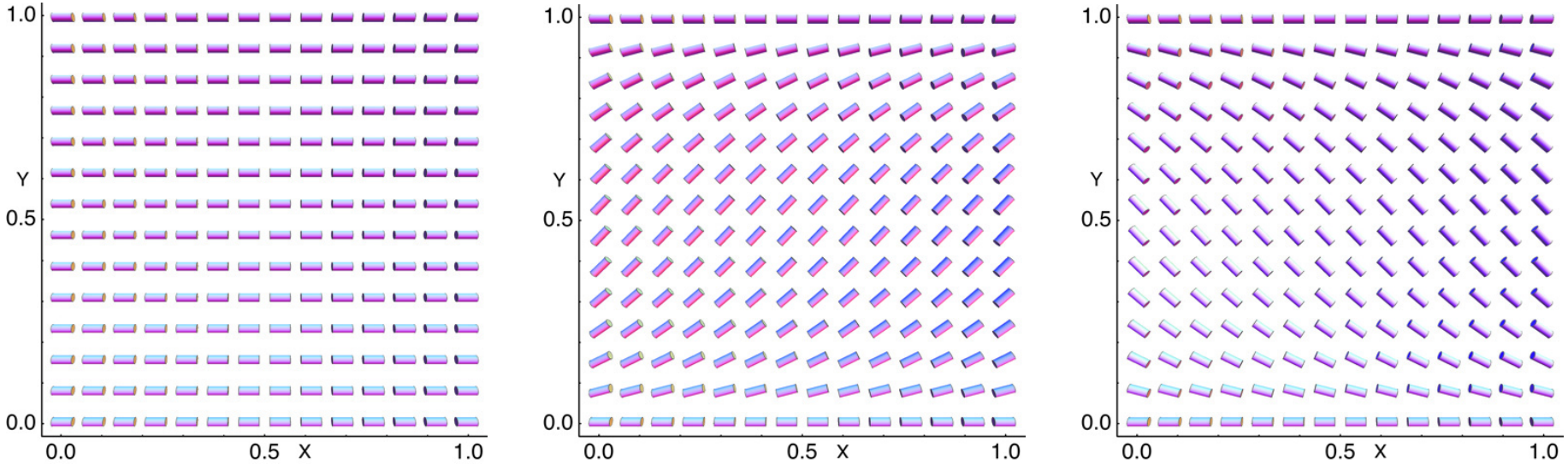
- n periodic in x and parallel to x-axis along $y = 0, y = 1$
- Frank constants $(K_1, K_2, K_3) = (1, 0.62903, 1.32258)$ (5CB)
- electric potential $\phi(x, 0) = 0, \phi(x, 1) = V$
- permittivity of free space $\epsilon_0 = 1.42809$
- perpendicular dielectric permittivity $\epsilon_\perp = 7$
- dielectric anisotropy $\epsilon_a = 11.5$

Application: Freedericksz transition



Bifurcation diagrams for maximum angular tilt and free energy as a function of V. The critical voltage is $V^* \approx 0.775$.

Application: Freedericksz transition



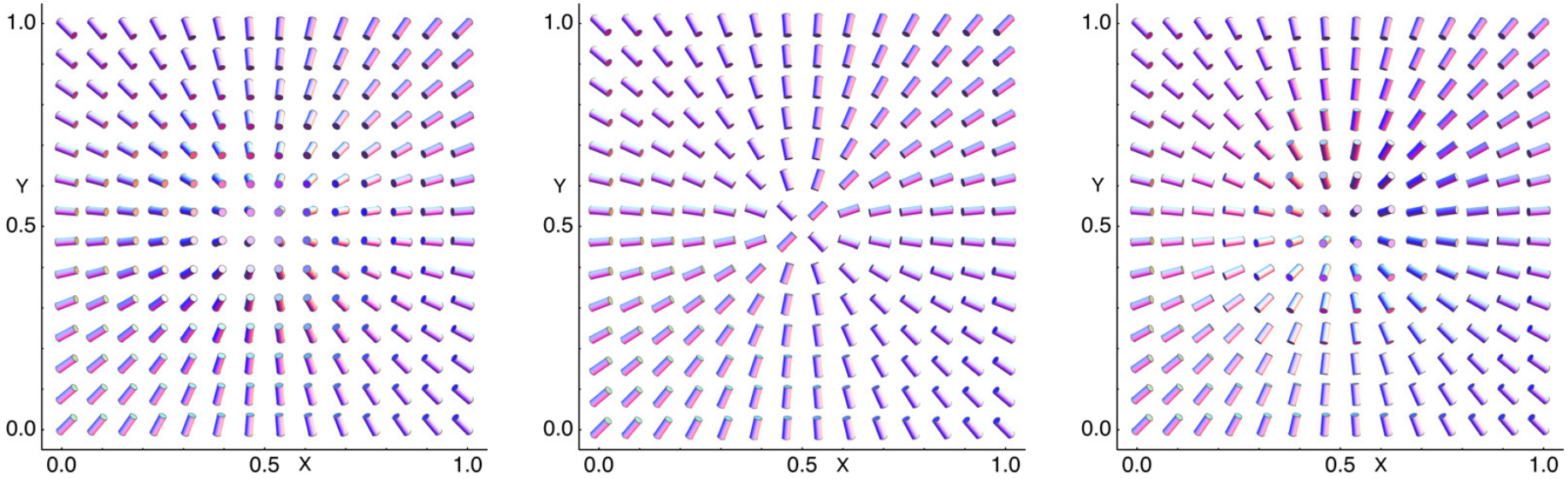
Three solutions for $V = 1.1$.

Application: escape and disclination solutions

Minimise Oseen–Frank energy on a unit square subject to

- n radial from the centre
- Frank constants $(K_1, K_2, K_3) = (1, 3, 1.2)$
- no electric field present

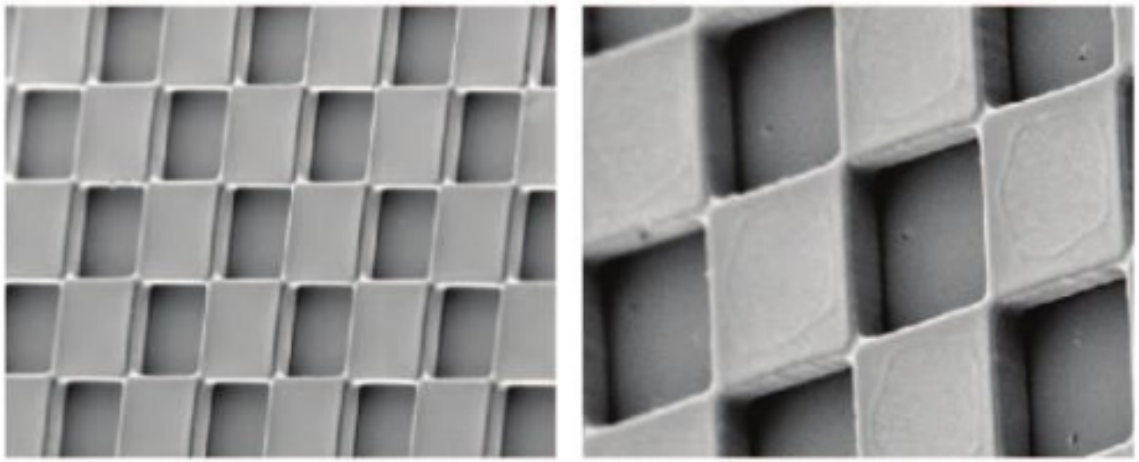
Application: escape and disclination solutions



Two escape and one disclination solution, with energies (9.971, 24.042, 9.971). The energy of the middle solution diverges with mesh refinement.

Application: square well filled with nematic LCs

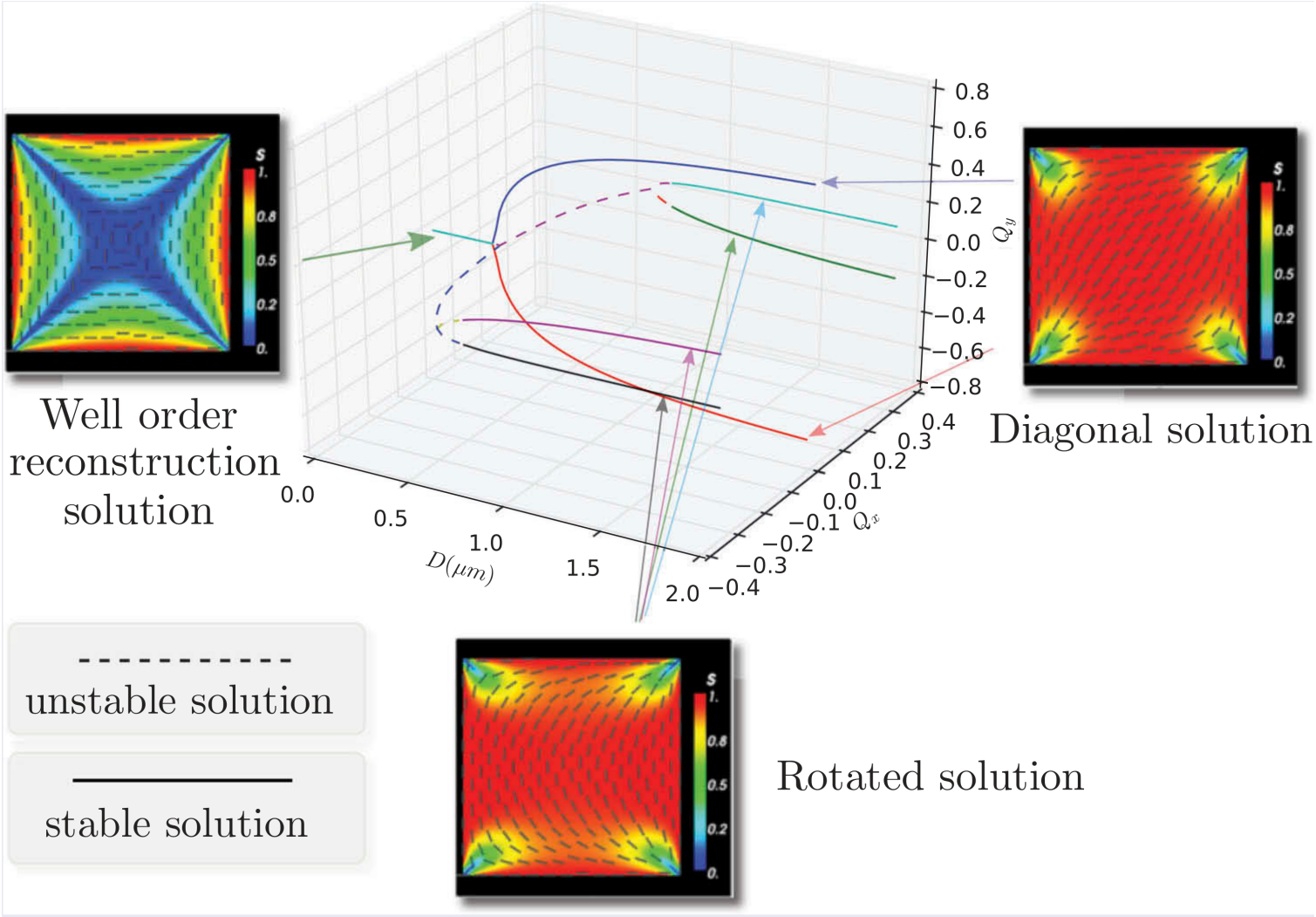
We consider the square wells filled with nematic liquid crystals considered by Tsakonas et al. (Appl. Phys. Lett, 2007) and Majumdar et al.



Minimise Landau–de Gennes energy on a square subject to

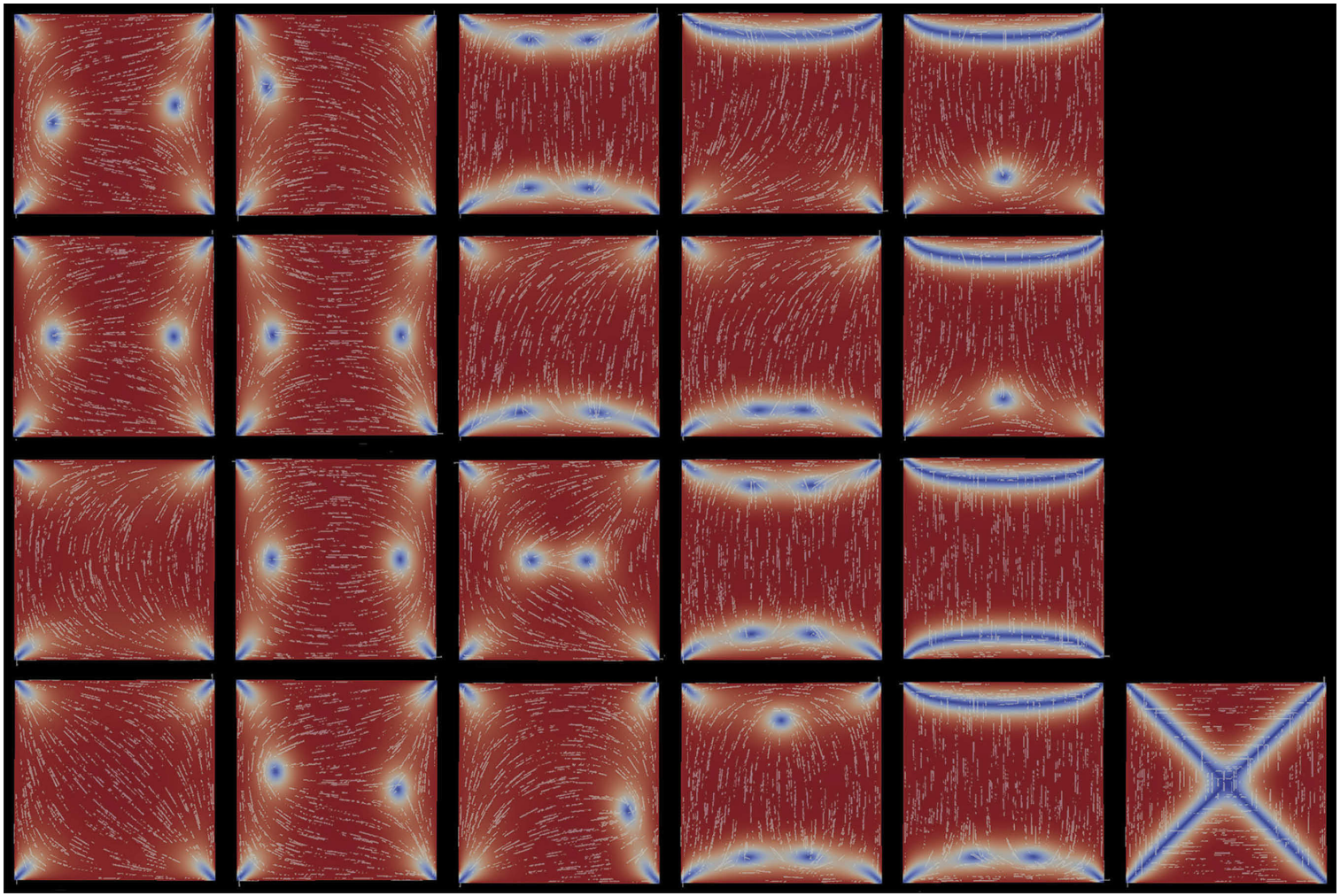
- $Q_{11} \geq 0$ on horizontal edges,
- $Q_{11} \leq 0$ on vertical edges,
- $Q_{12} = 0$ on $\partial\Omega$.

Application: square well filled with nematic LCs



Bifurcation diagram showing stable states as a function of square edge length D.

Application: square well filled with nematic LCs



21 different stationary points, coloured by the order parameter, for $D = 1.5\,\mu\mathrm{m}$.

Application: geometrically frustrated cholesteric

Description

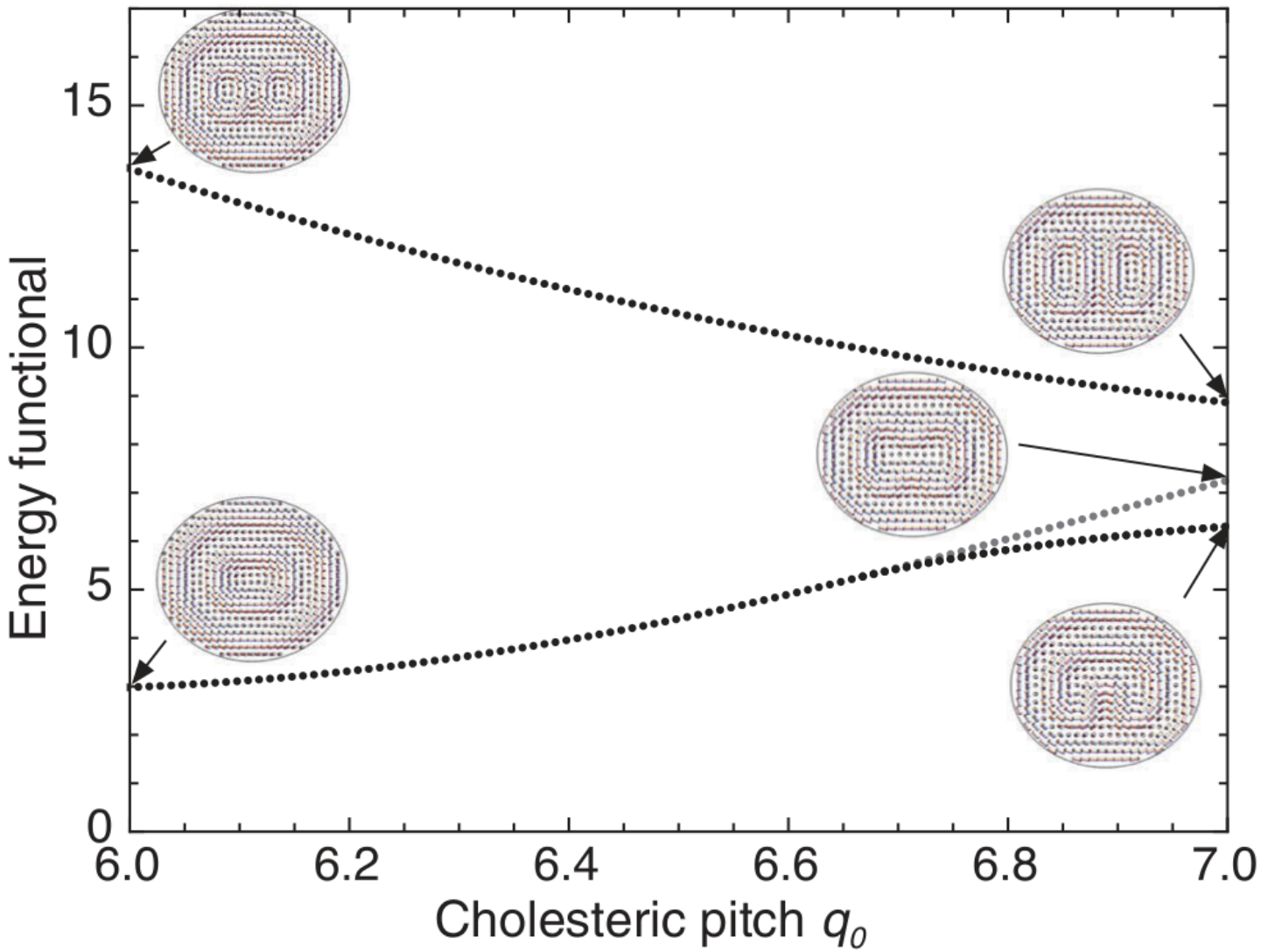
In the absence of boundaries, the cholesteric adopts a helical structure with a preferred pitch q_0. On an ellipse, the boundary conditions preclude the energetically preferred uniformly twisted state. This frustration is resolved by deformation of the cholesteric layers or the introduction of defects, in multiple ways.

Minimise Oseen–Frank energy with cholesteric term in an ellipse subject to

- $n = (0, 0, 1)$ on the boundary
- Frank constants $(K_1, K_2, K_3) = (1, 3.2, 1.1)$
- no electric field

as a function of cholesteric pitch q_0.

Application: geometrically frustrated cholesteric



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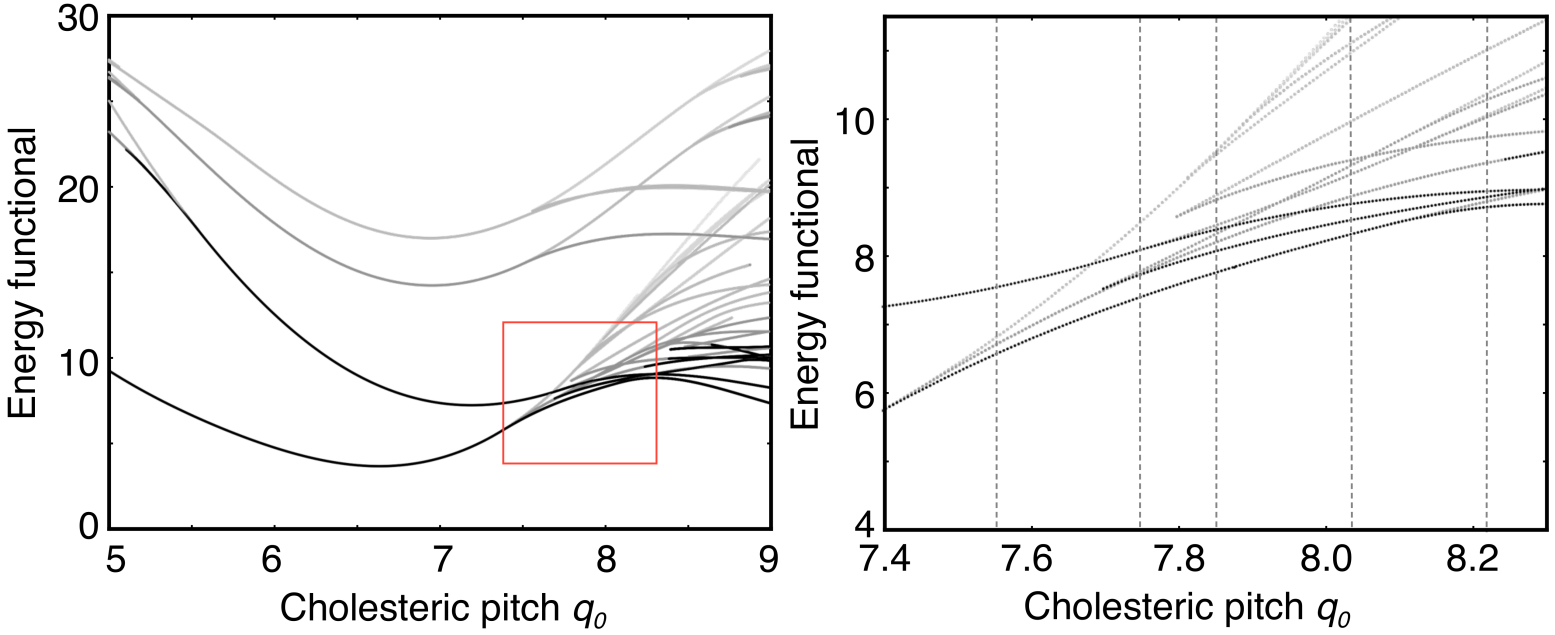

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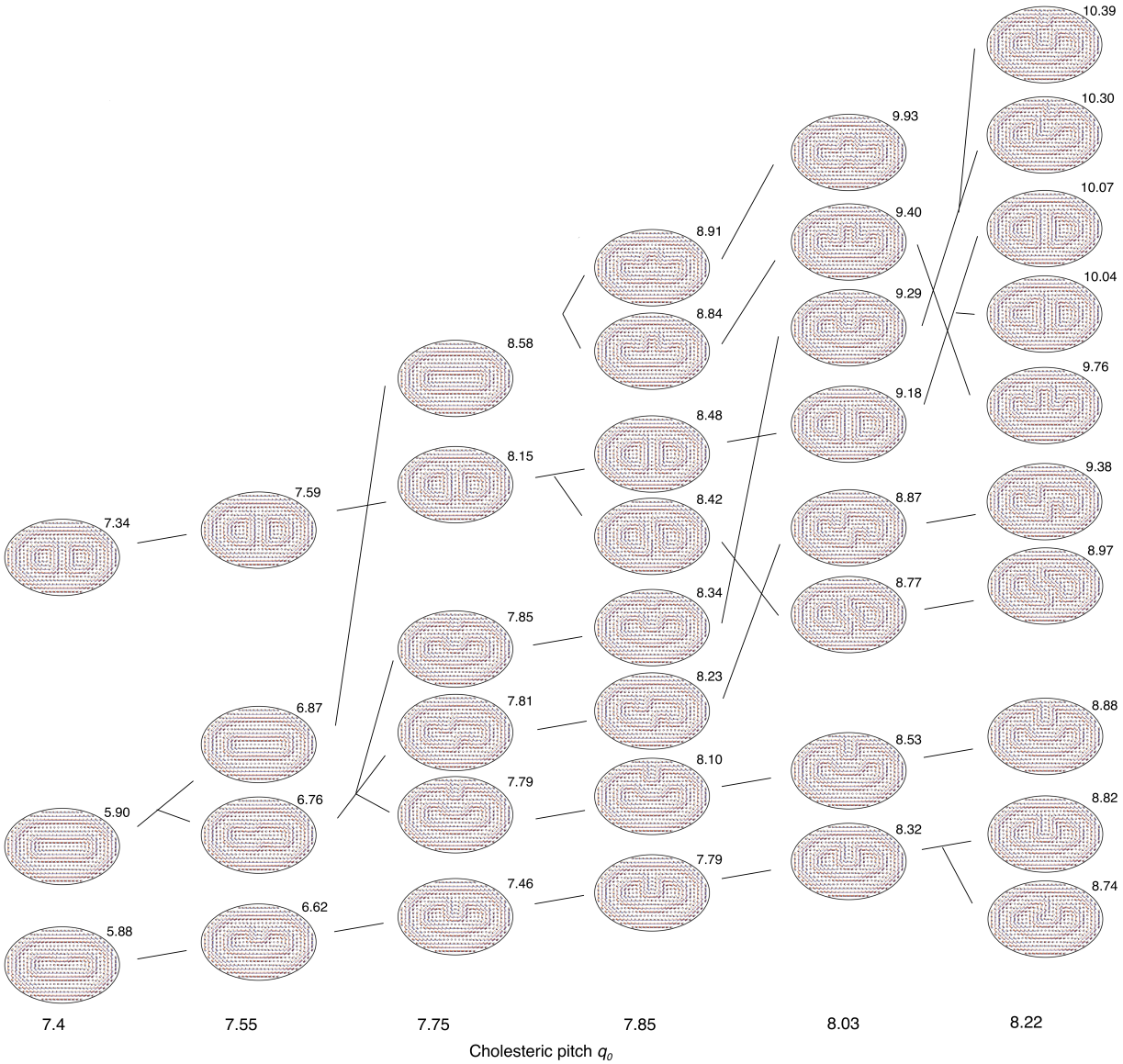

Application: smectic-A

Pevnyi–Selinger–Sluckin (2014) model

Minimise

$$J(n) = \int_\Omega \frac{a}{2}\delta\rho^2 + \frac{c}{4}\delta\rho^4 + B\left|\nabla\nabla\delta\rho + q^2\mathbf{n}\otimes\mathbf{n}\delta\rho\right|^2 + \frac{K}{2}\left|\nabla\mathbf{n}\right|^2 \,\mathrm{d}x$$

subject to $\mathbf{n}\cdot\mathbf{n} = 1$, periodic in x, Dirichlet on $\mathbf{n}$ for $y \in \{0, 1\}$.

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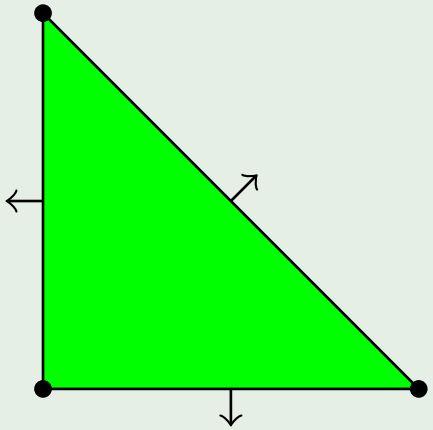
Solution: nonconforming Morley element



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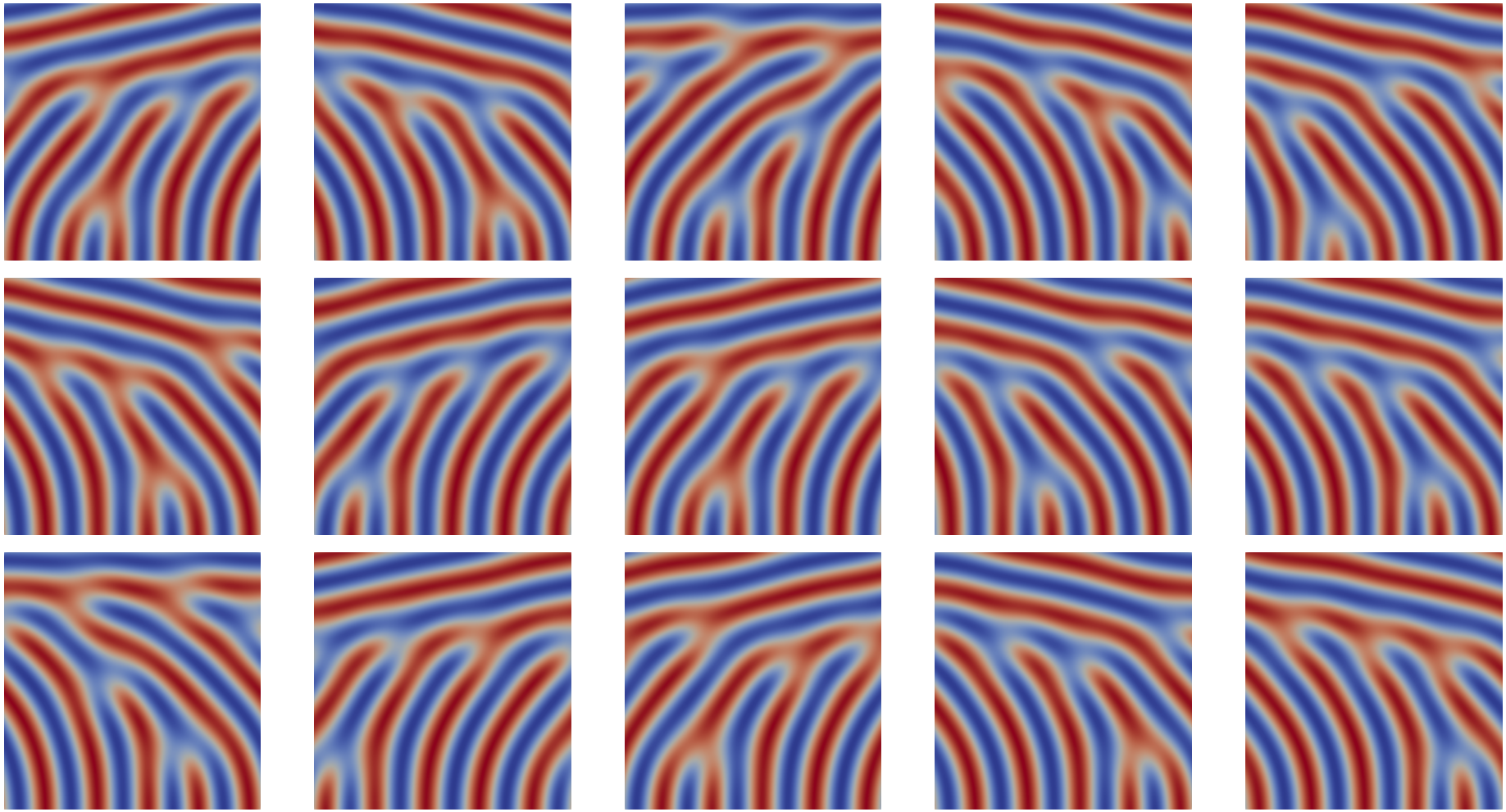

$\delta\rho$ for some of 73 solutions found for $q = 30, a = -10, c = 10, B = 10^{-5}, K = 0.3$.

Conclusions

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- Deflated problems can be **solved efficiently**.