Computing disconnected bifurcation diagrams of partial differential equations

P. E. Farrell[1]

S. P. MacLachlan, T. J. Atherton, M. Robinson, A. Majumdar, R. Erban, ...

[1]University of Oxford

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Section 1

Introduction

Can you conduct an experiment twice . . .

and get two different answers?

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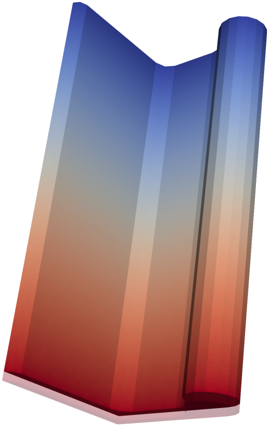
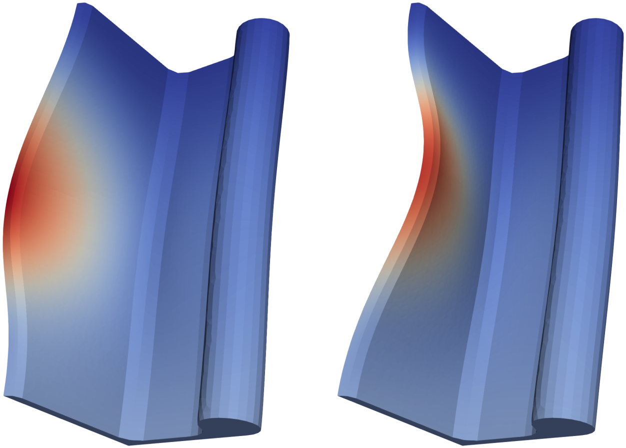


Axial displacement test of an Embraer aircraft stiffener.

Can you conduct an experiment twice ...

and get two different answers?



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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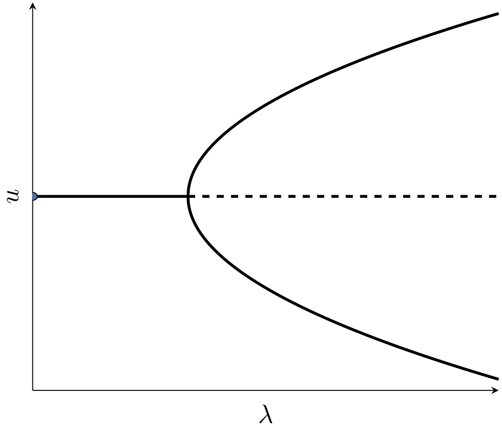
Today

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

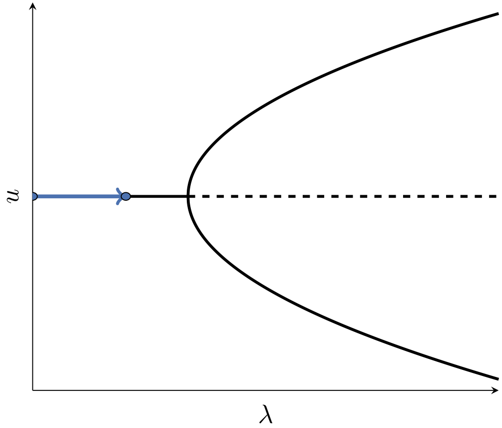
Section 2

The classical algorithm

Branch switching

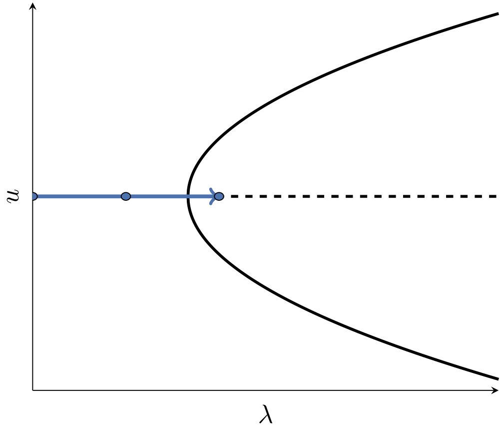


Branch switching



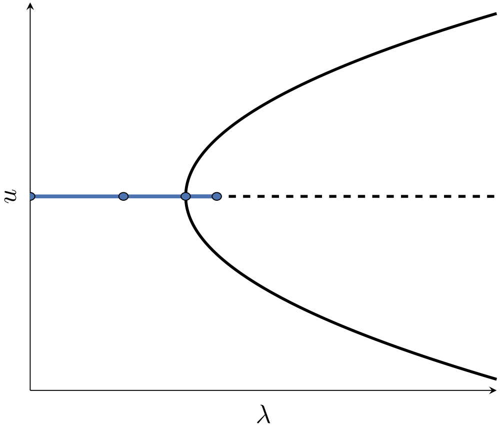
Step I: continuation

Branch switching



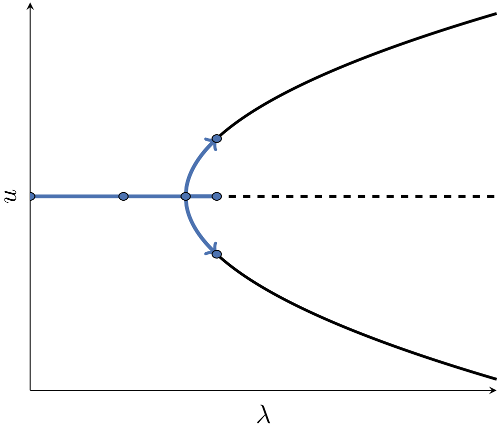
Step II: continuation

Branch switching



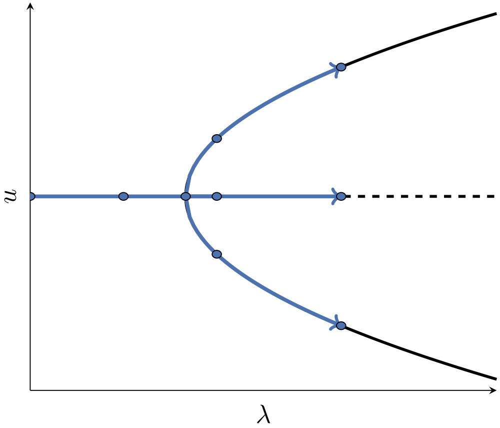
Step III: detect bifurcation point

Branch switching



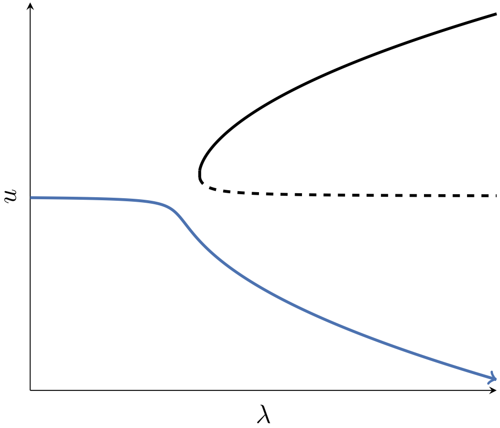
Step IV: compute eigenvectors and switch

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**.

This work

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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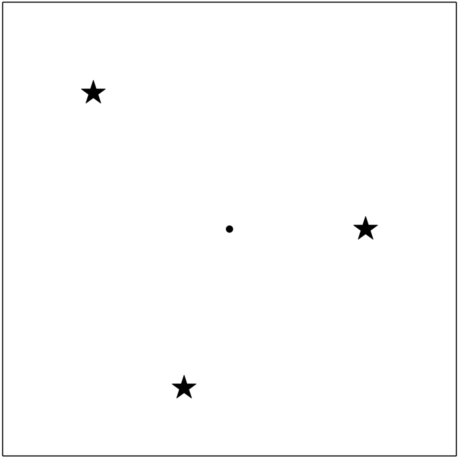
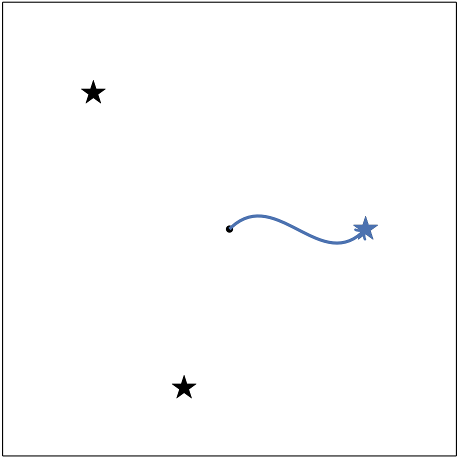
Find more solutions, starting from the same initial guess.

Finding many solutions from the same guess

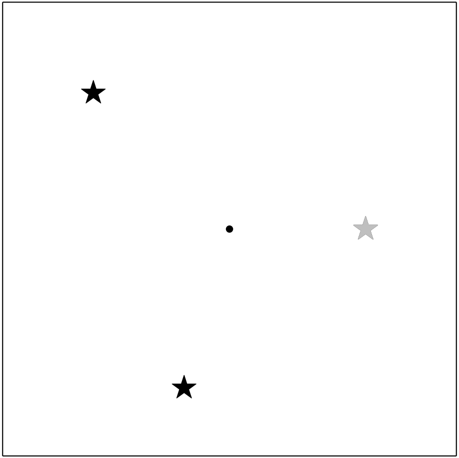


Finding many solutions from the same guess



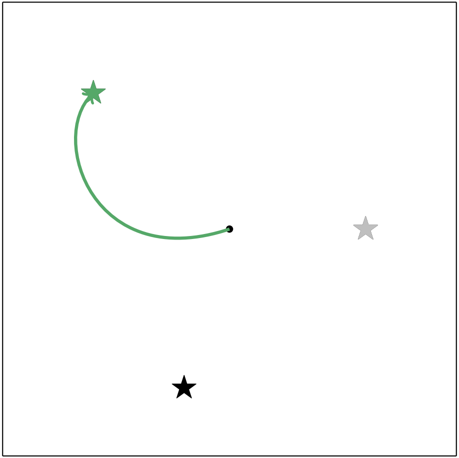
Step I: Newton from initial guess

Finding many solutions from the same guess



Step II: deflate solution found

Finding many solutions from the same guess



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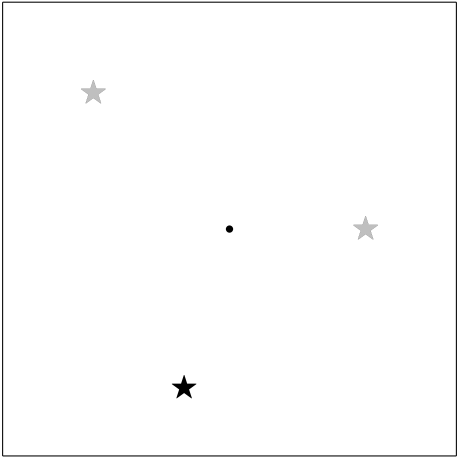

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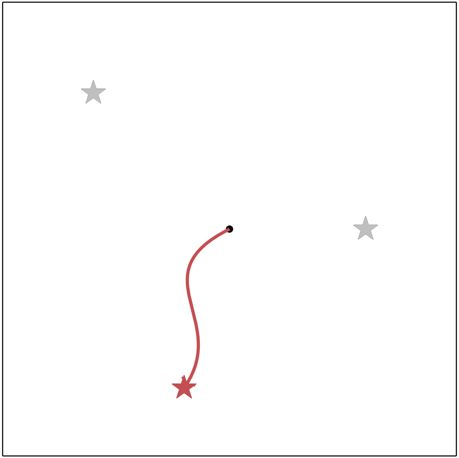

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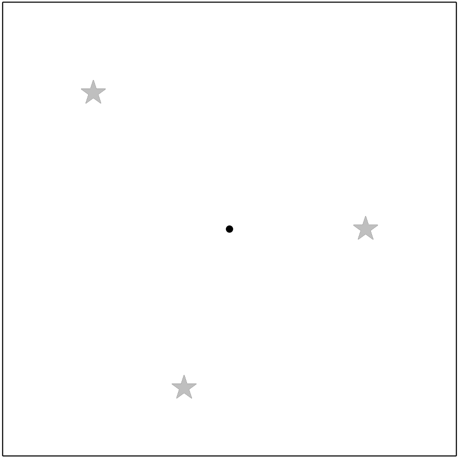

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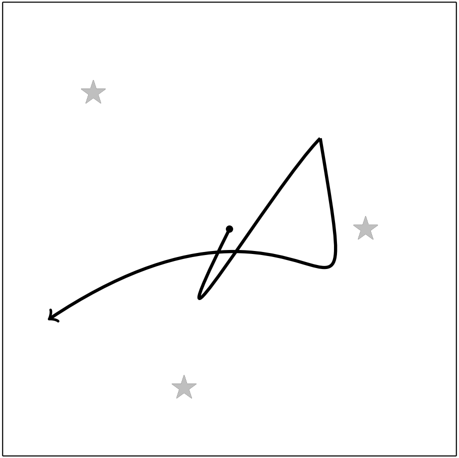

Step III: termination on nonconvergence

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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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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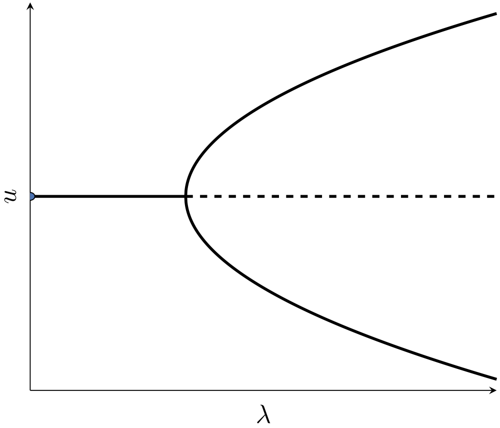
Theorem (F., Birkisson, Funke, 2014)

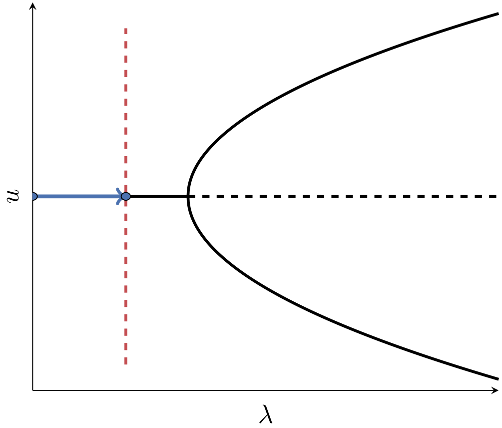
This is a deflation operator for $p \geq 1$:

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

Deflated continuation

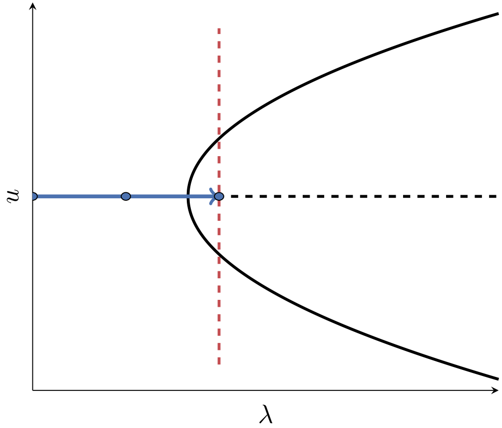


Deflated continuation



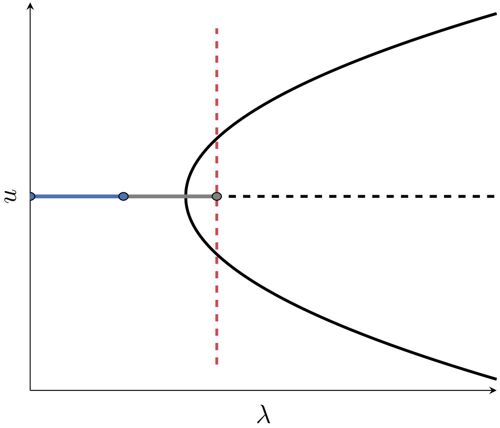
Step I: continuation

Deflated continuation



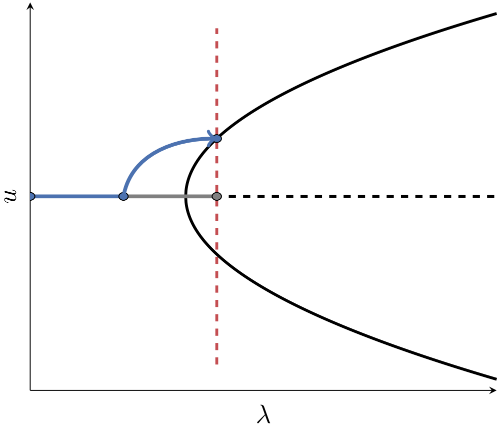
Step II: continuation

Deflated continuation



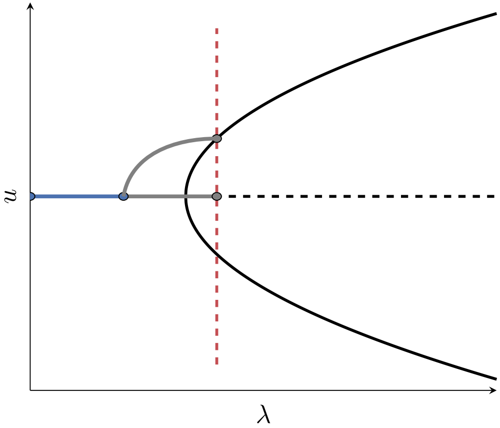
Step III: deflate

Deflated continuation



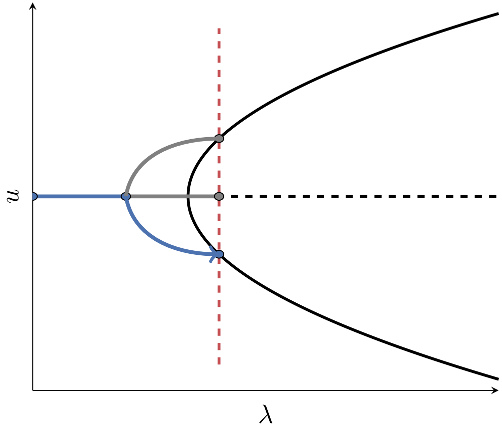
Step III+: solve deflated problem

Deflated continuation



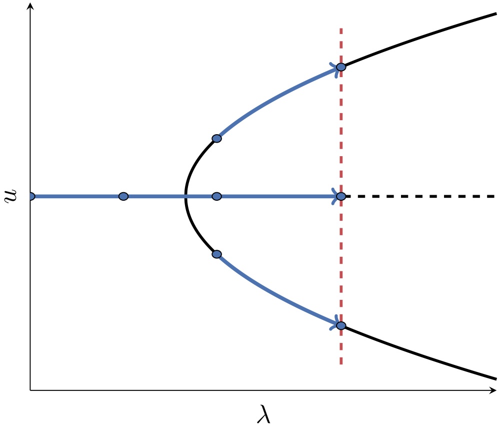
Step III: deflate

Deflated continuation



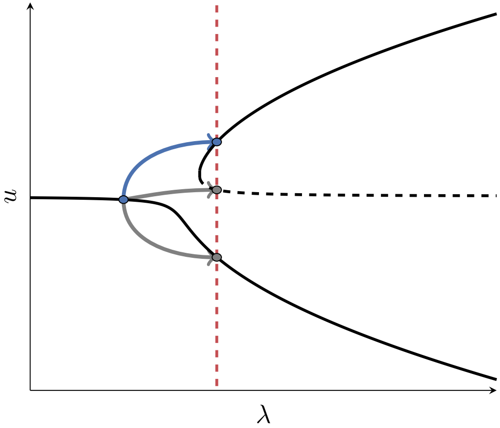
Step III+: solve deflated problem

Deflated continuation



Step IV: continuation on branches

Deflated continuation



A disconnected diagram.

Section 4

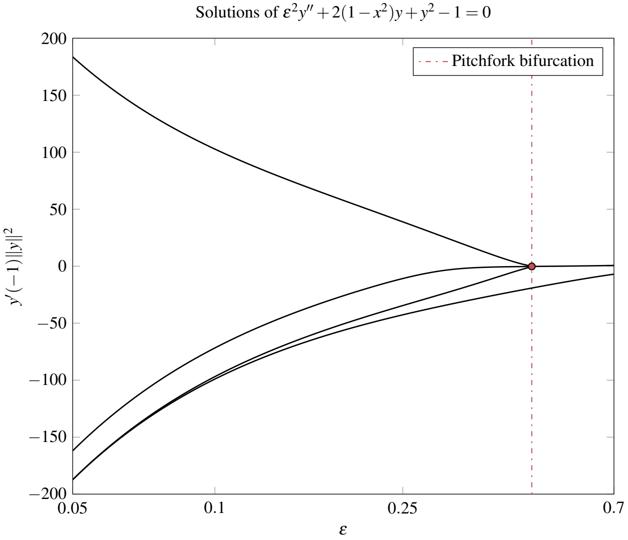
Applications

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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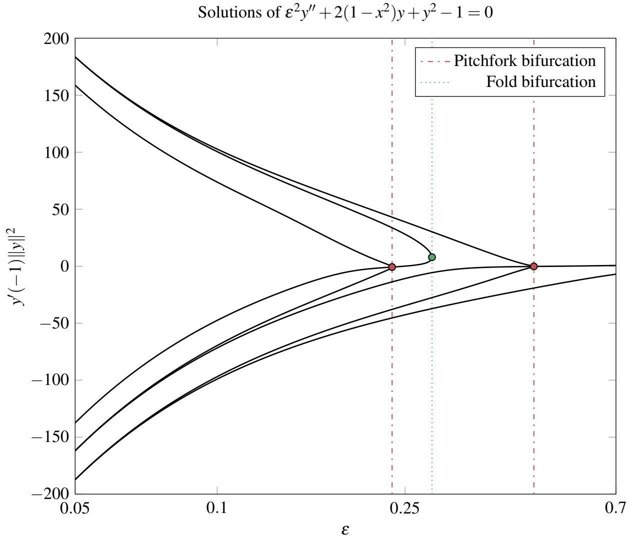

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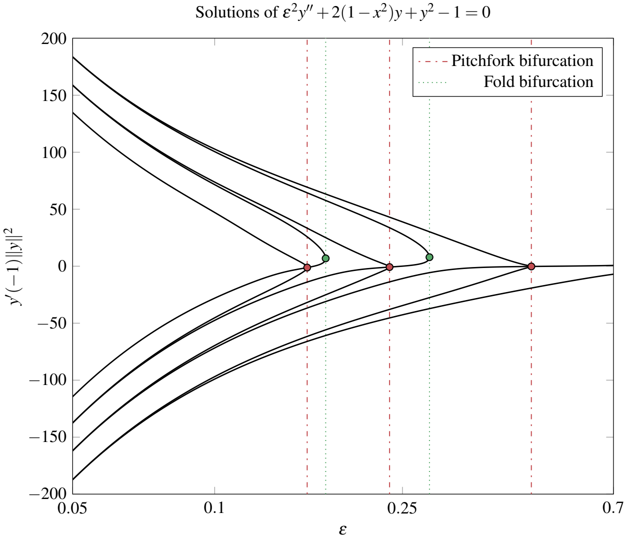

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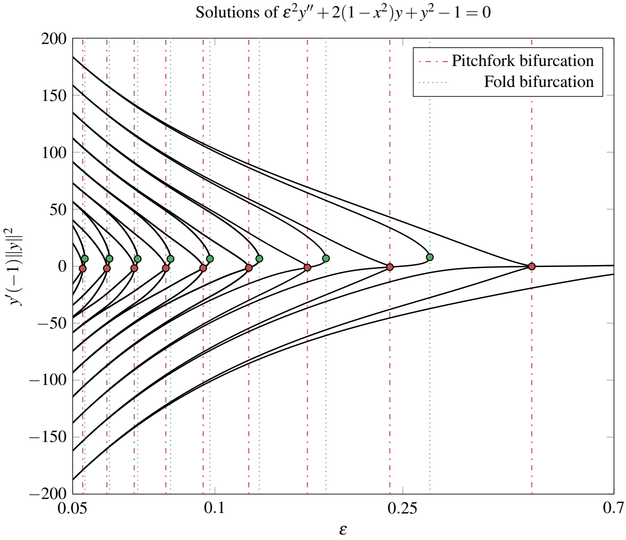

Application: Carrier's problem

Pitchfork bifurcations

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

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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%

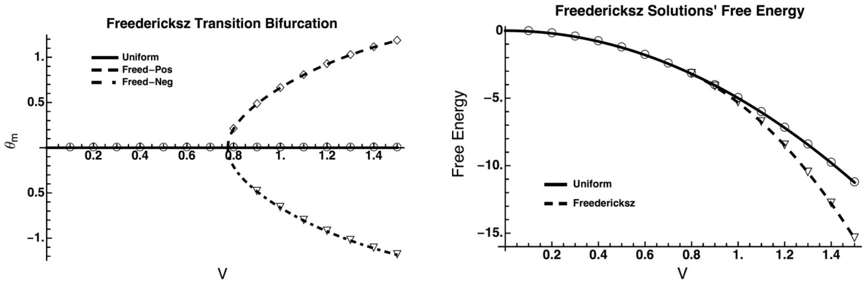
Computed and estimated parameter values for the first four fold bifurcations.

Application: Freedericksz transition

Minimise Frank–Oseen energy on a unit square subject to

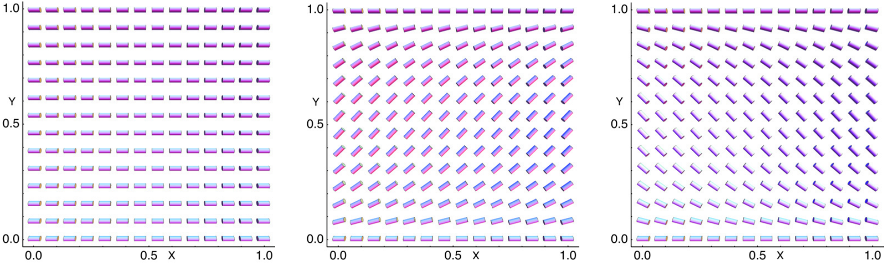
- n periodic in x and parallel to x-axis along $y = 0, y = 1$
- Frank constants $(K_1, K_2, K_3) = (1, 0.62903, 1.32258)$ (5CB)
- electric potential $\phi(x, 0) = 0, \phi(x, 1) = V$
- permittivity of free space $\epsilon_0 = 1.42809$
- perpendicular dielectric permittivity $\epsilon_\perp = 7$
- dielectric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



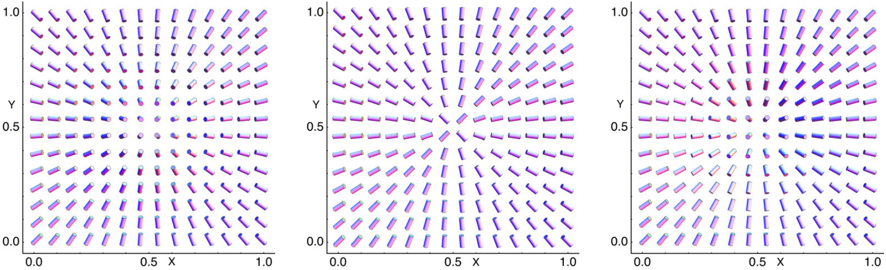
Three solutions for $V = 1.1$.

Application: escape and disclination solutions

Minimise Frank–Oseen 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



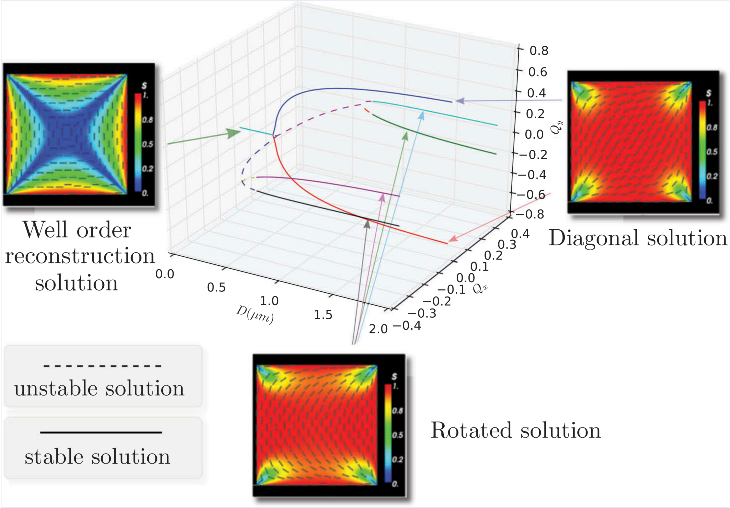
Two escape and one disclination solution, with energies (9.971, 24.042, 9.971). The energy of the middle solution diverges with mesh refinement.

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).
Minimise Landau–de Gennes energy on a square subject to

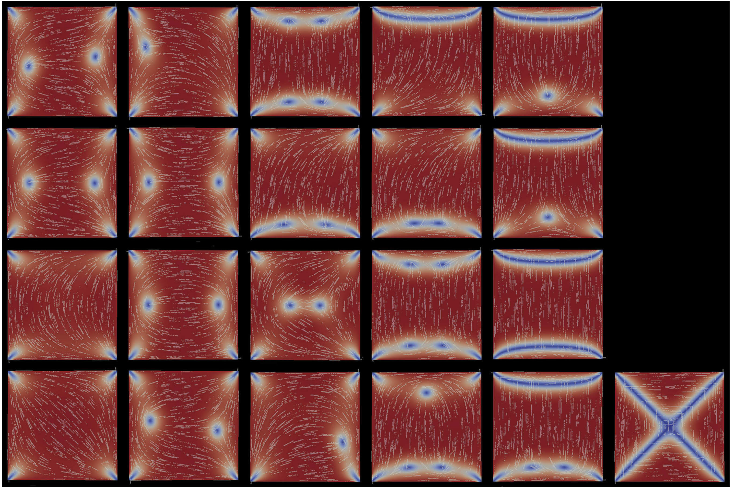
- $Q_{11} \geq 0$ on horizontal edges
- $Q_{11} \leq 0$ on vertical edges
- $Q_{12} = 0$ on $\partial\Omega$

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 $D = 1.5\,\mu\text{m}$.

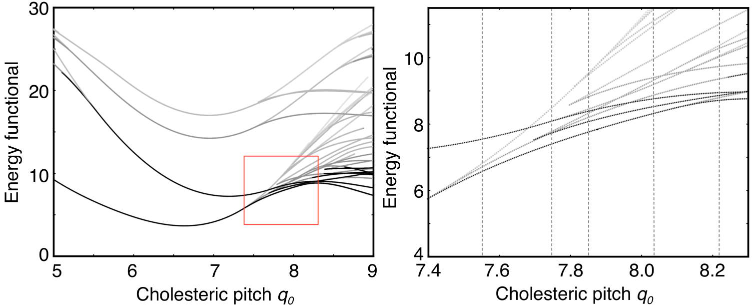
Application: cholesteric liquid crystals

Minimise Frank–Oseen 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: cholesteric liquid crystals



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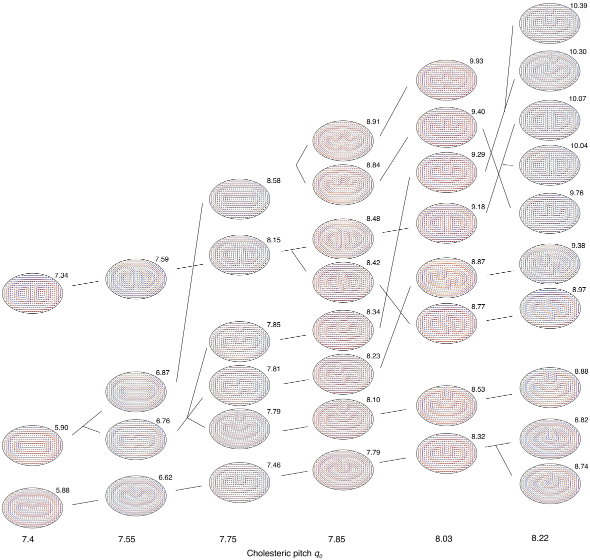

Conclusions

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- Multiple solutions of PDEs are ubiquitous and important.
- Deflation is a powerful and useful technique.
- Deflated problems can be solved efficiently.
- There are **interesting applications** in liquid crystals.

Section 6

Symmetries

Symmetries

Nonisolated solutions

What if the equation has a continuous symmetry group?

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Nonisolated solutions

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Philosophy

The fundamental structures are the distinct **orbits** of solutions.

Symmetries

Nonisolated solutions

What if the equation has a continuous symmetry group?

Philosophy

The fundamental structures are the distinct **orbits** of solutions.

Key idea

Construct a deflation operator that respects the Lie group.

Application: Bose–Einstein condensates

Stationary Gross–Pitaevskii equation

$$-\frac{1}{2}\Delta\phi + V(x^2+y^2)\phi - \mu\phi + |\phi|^2\phi = 0, \qquad \phi|_{\partial\Omega} = 0.$$

Application: Bose–Einstein condensates

Stationary Gross–Pitaevskii equation

$$-\frac{1}{2}\Delta\phi + V(x^2+y^2)\phi - \mu\phi + |\phi|^2\phi = 0, \qquad \phi|_{\partial\Omega} = 0.$$

First symmetry group $\mathrm{SO}(2)$

$$\phi(x,y) \mapsto e^{i\theta}\phi(x,y), \quad \theta \in \mathbb{R}.$$

Application: Bose–Einstein condensates

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Resulting deflation operator

$$M(\psi,\phi) = \left\| |\phi|^2 - |\psi|^2 \right\|^{-2} + 1.$$

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Second symmetry group $\mathrm{SO}(2)$

$$\phi(x,y) \mapsto \phi(x\cos\theta - y\sin\theta, x\sin\theta + y\cos\theta), \quad \theta \in \mathbb{R}.$$

Application: Bose–Einstein condensates

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Second symmetry group $\mathrm{SO}(2)$

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Resulting deflation operator

$$M(\psi,\phi) = \left\|\tilde{\phi} - \tilde{\psi}\right\|^{-2} + 1,$$

where

$$\tilde{\psi}(x,y) := \frac{1}{2\pi}\int_0^{2\pi} \psi(x\cos\theta - y\sin\theta, x\sin\theta + y\cos\theta)\ \mathrm{d}\theta.$$

Application: Bose–Einstein condensates

Stationary Gross–Pitaevskii equation

$$-\frac{1}{2}\Delta\phi + V(x^2+y^2)\phi - \mu\phi + |\phi|^2\phi = 0, \qquad \phi|_{\partial\Omega} = 0.$$

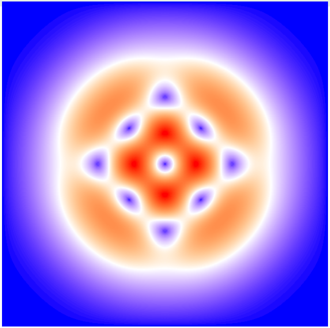
Final deflation operator

$$M(\psi,\phi) = \left\| \widetilde{|\phi|^2} - \widetilde{|\psi|^2} \right\|^{-2} + 1.$$

Application: Bose–Einstein condensates

Stationary Gross–Pitaevskii equation

$$-\frac{1}{2}\Delta\phi + V(x^2 + y^2)\phi - \mu\phi + |\phi|^2\phi = 0, \qquad \phi|_{\partial\Omega} = 0.$$

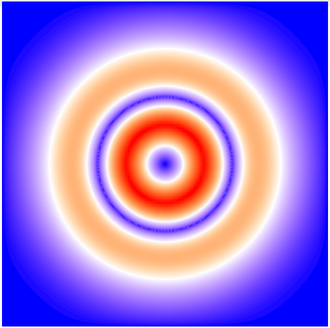


Some of 21 distinct orbits of the Gross–Pitaevskii equation, $\mu = 1.3$.

Application: Bose–Einstein condensates

Stationary Gross–Pitaevskii equation

$$-\frac{1}{2}\Delta\phi + V(x^2+y^2)\phi - \mu\phi + |\phi|^2\phi = 0, \qquad \phi|_{\partial\Omega} = 0.$$



Some of 21 distinct orbits of the Gross–Pitaevskii equation, $\mu = 1.3$.

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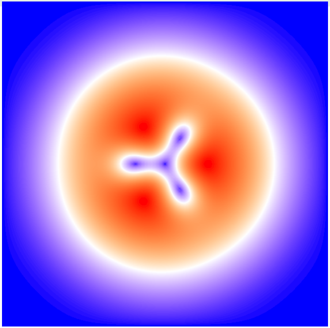

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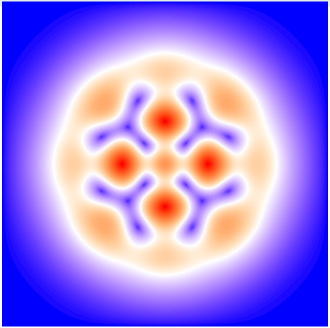

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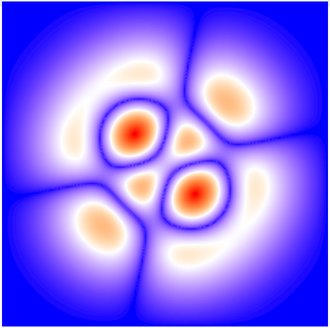

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Headline result

These orbits were discovered with (almost) **no user-supplied data**.