Computing disconnected bifurcation diagrams 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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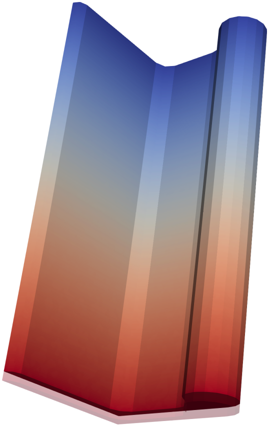
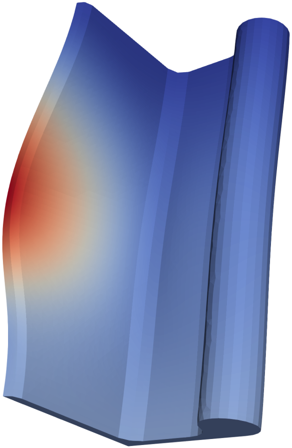


Axial displacement test of an Embraer aircraft stiffener.

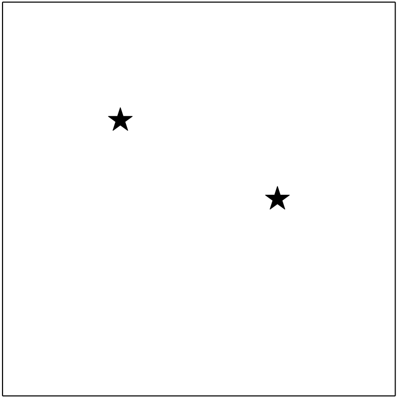
Can you conduct an experiment twice . . .

and get two different answers?



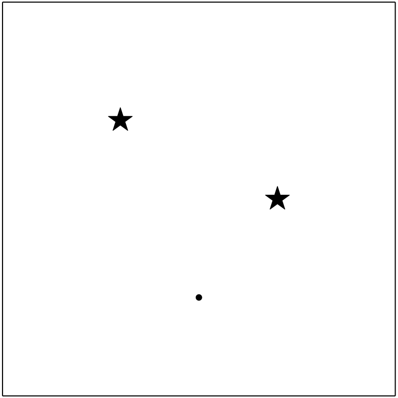
Two different, stable configurations.

Why worry?



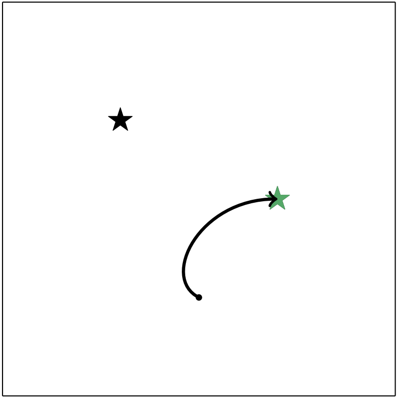
A PDE with two unknown solutions

Why worry?



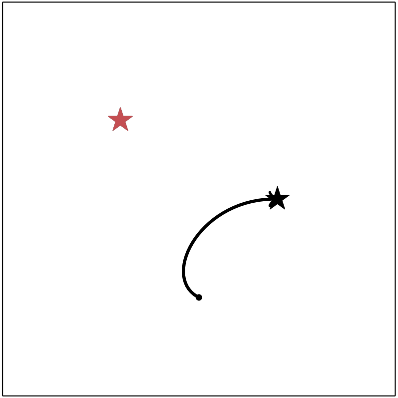
Start from some initial guess

Why worry?



We converge to one solution, our prediction

Why worry?



But nature has chosen another (unknown) solution!

Mathematical formulation

Compute the multiple *solutions* u of an equation

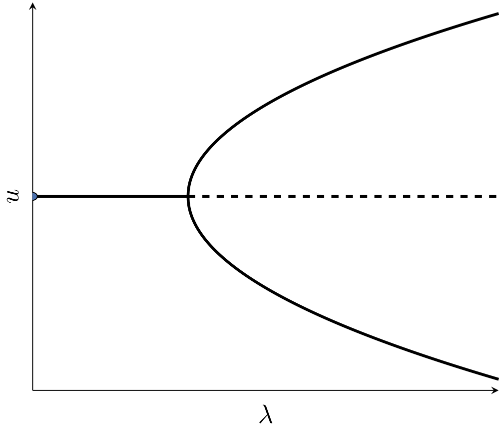
$$f(u, \lambda) = 0$$
$$f : V \times \mathbb{R} \to V^*$$

as a function of a parameter λ.

Section 2

The classical algorithm

Branch switching



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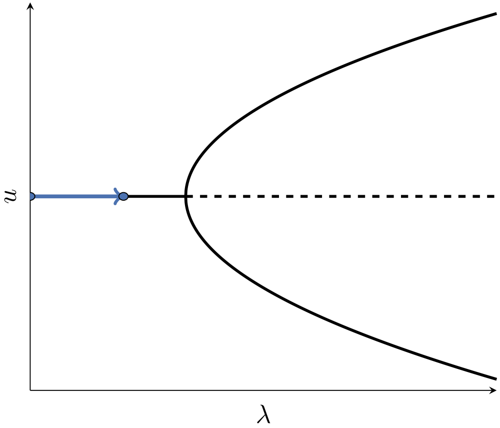
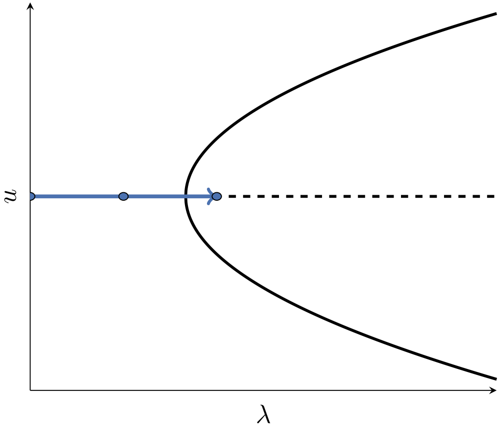


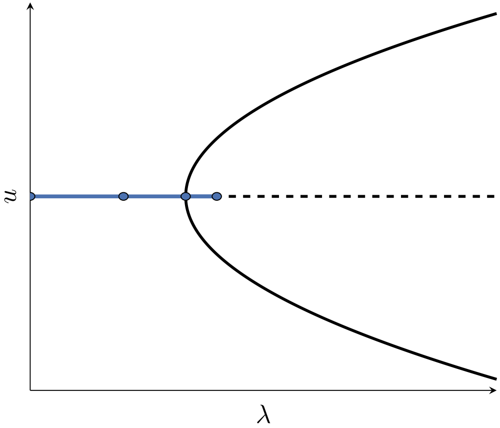
Step I: continuation

Branch switching



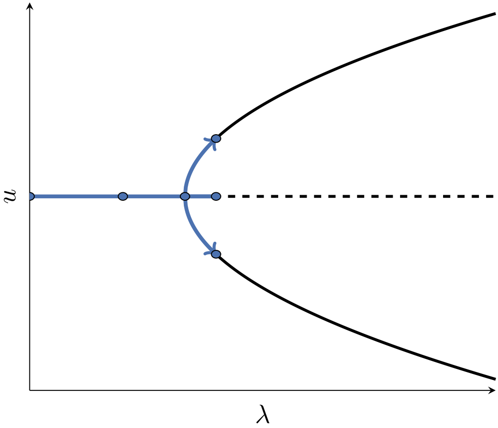
Step II: continuation

Branch switching



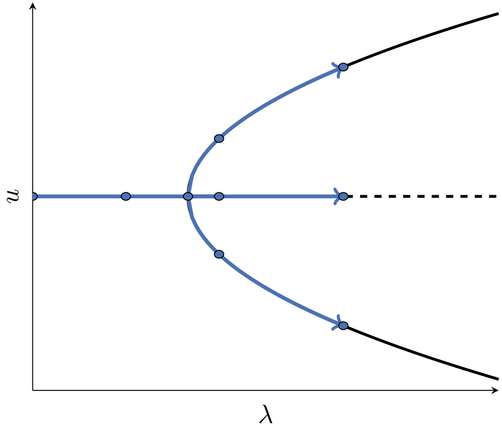
Step III: detect bifurcation point

Branch switching



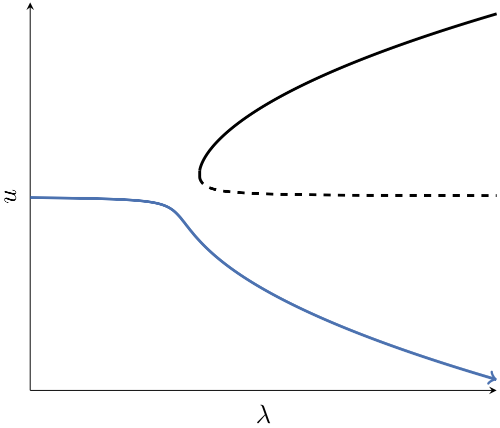
Step IV: compute eigenvectors and switch

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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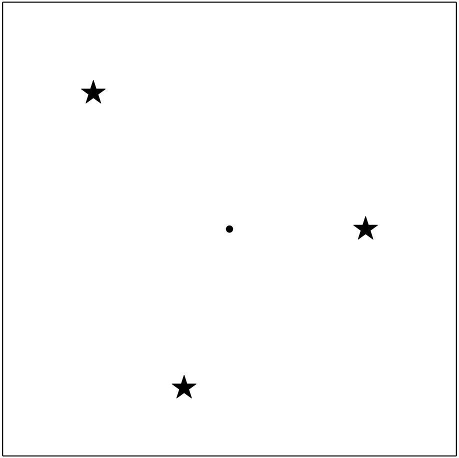
Find more solutions, starting from the same initial guess.

Finding many solutions from the same guess



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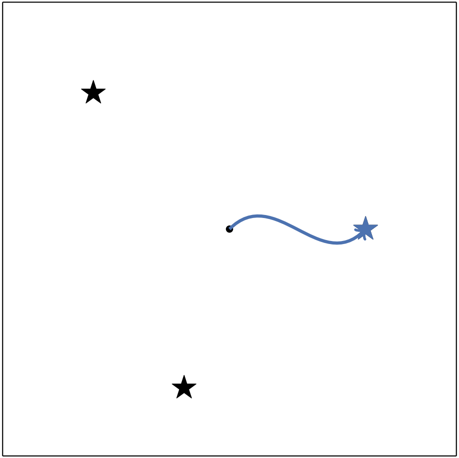
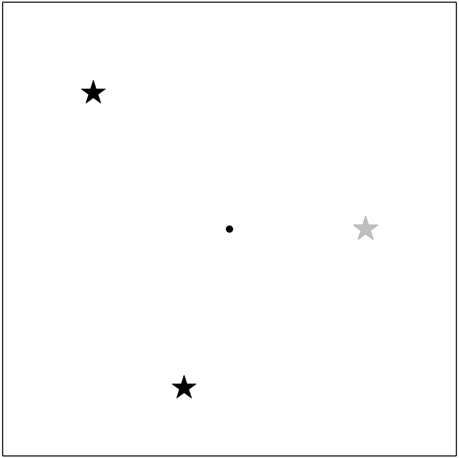


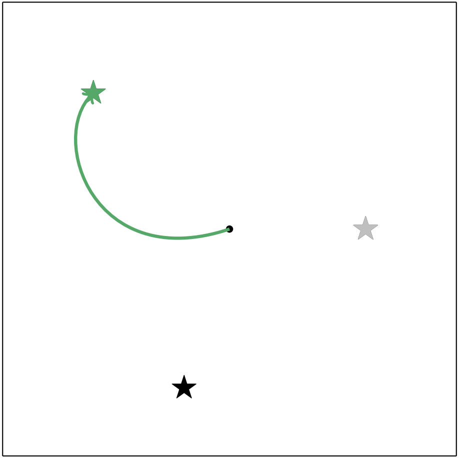
Step I: Newton from initial guess

Finding many solutions from the same guess



Step II: deflate solution found

Finding many solutions from the same guess



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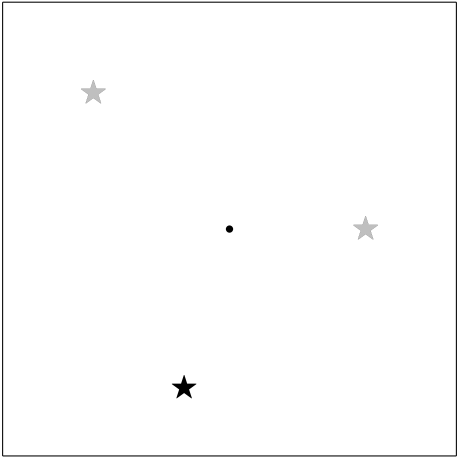

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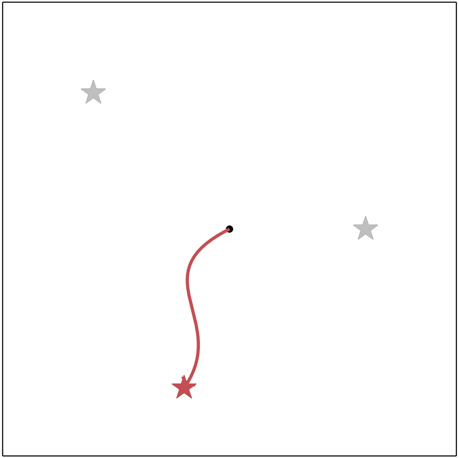

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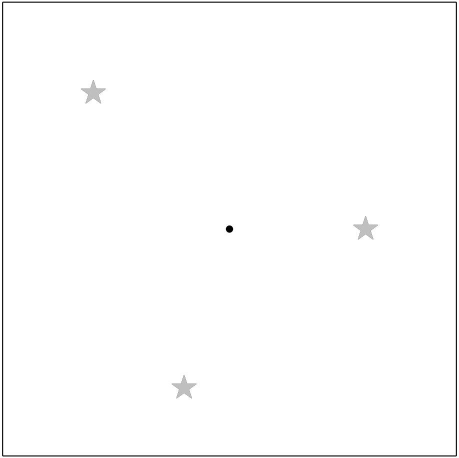

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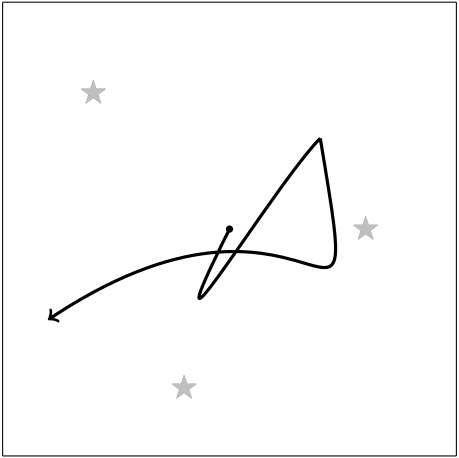
Finding many solutions from the same guess



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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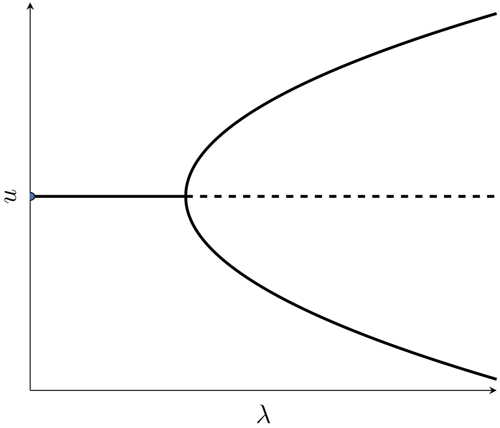
Theorem (F., Birkisson, Funke, 2014)

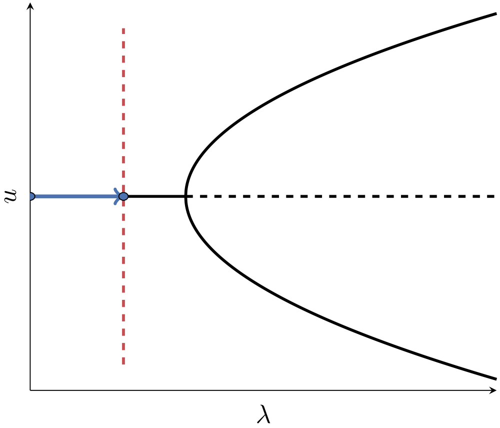
This is a deflation operator for $p \geq 1$:

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

Deflated continuation

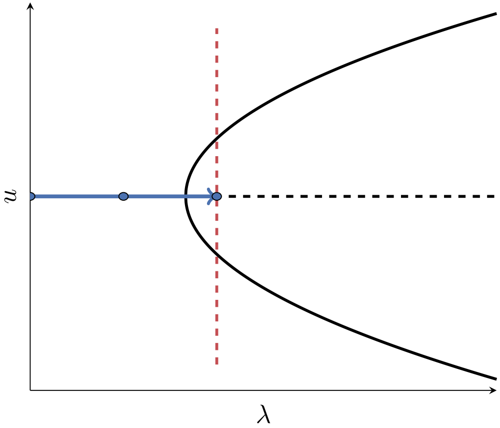


Deflated continuation



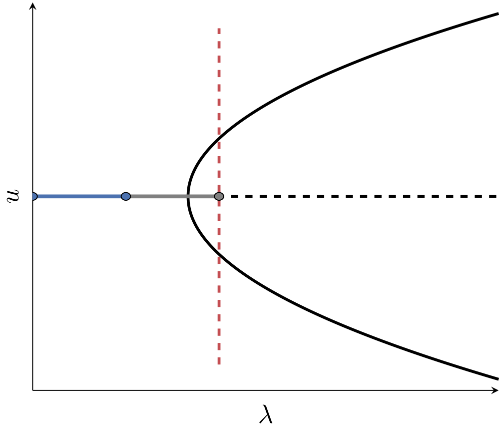
Step I: continuation

Deflated continuation



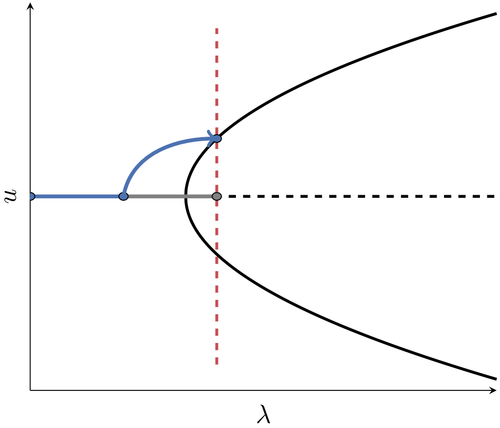
Step II: continuation

Deflated continuation



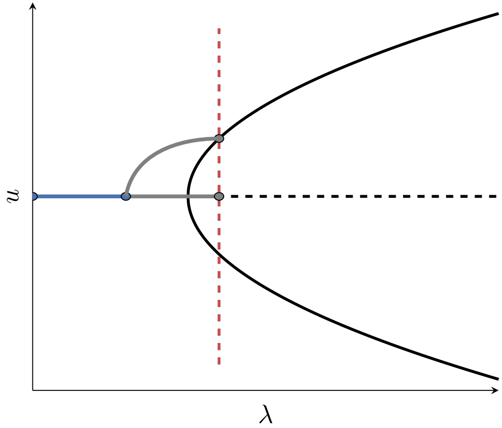
Step III: deflate

Deflated continuation



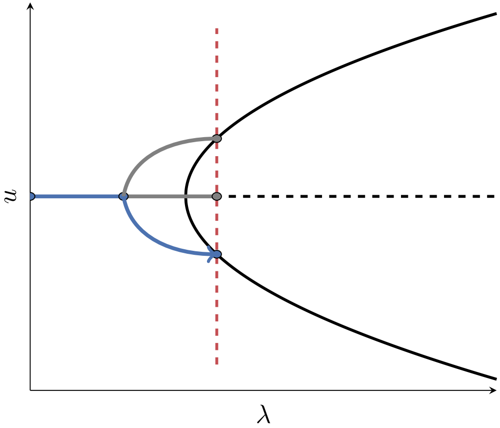
Step III+: solve deflated problem

Deflated continuation



Step III: deflate

Deflated continuation



Step III+: solve deflated problem

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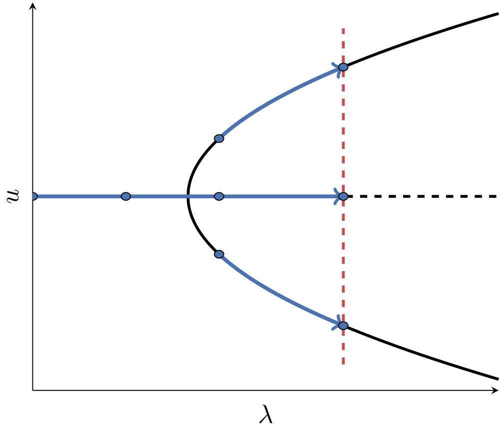
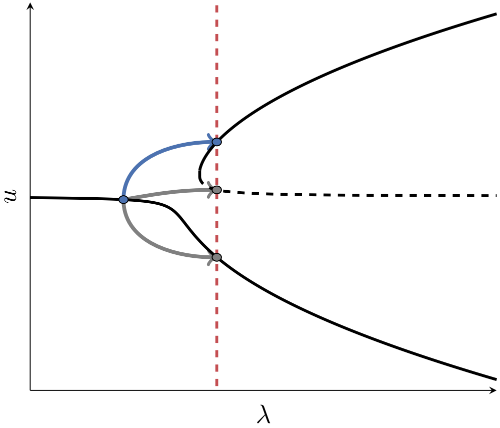


Step IV: continuation on branches

Deflated continuation



A disconnected diagram.

An example: the winged cusp

The winged cusp for $x \in \mathbb{R}$

$$f(x, \lambda) = x^3 - 2\lambda x + \lambda^2 - 2\lambda + 1 = 0$$

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

$$J_G(u) = M(u;r)J_F(u) + F(u)M'(u;r)^\top$$

Newton–Krylov

A Newton step

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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

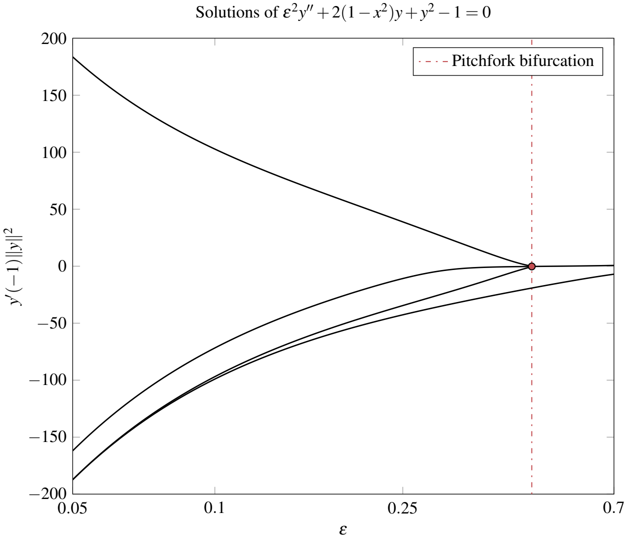
Applications

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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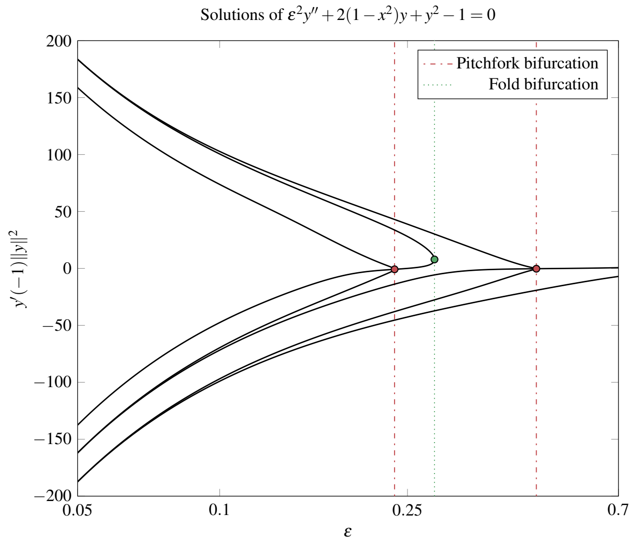

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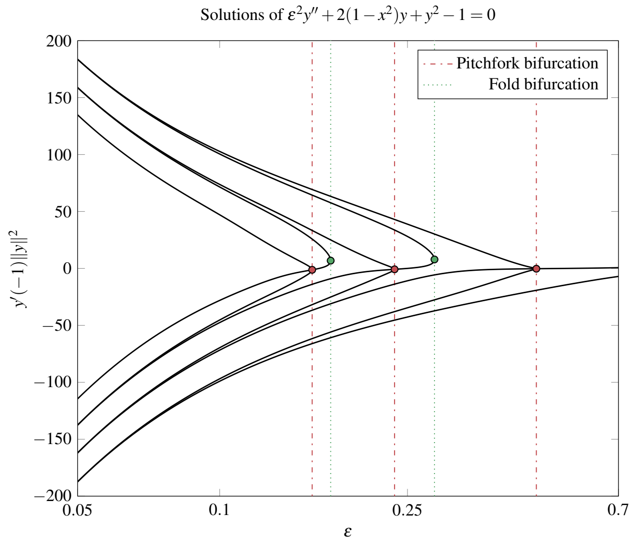

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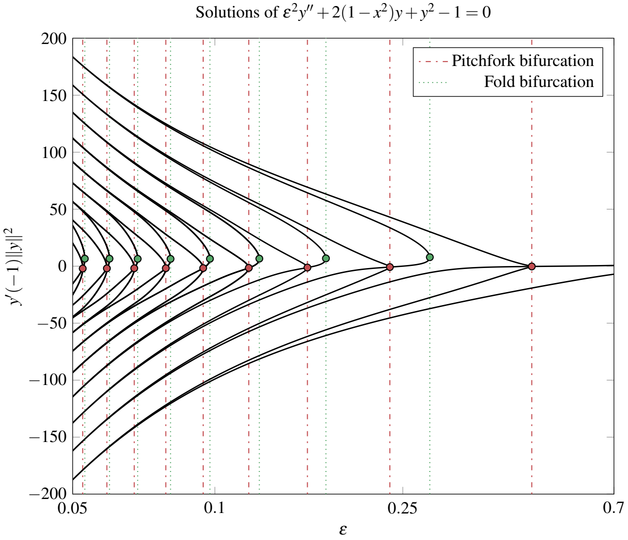


Application: Carrier's problem

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

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

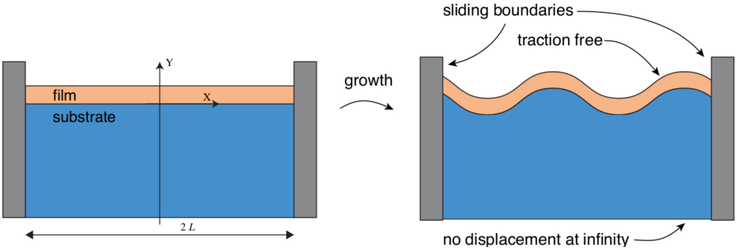
Connected component	Computed ε	Asymptotic estimate	Relative error
2	0.28522538	0.298545	4.670%
3	0.17186970	0.173608	1.011%
4	0.12421206	0.124634	0.3397%
5	0.09762446	0.0977706	0.1497%

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

Application: wrinkling of elastic bilayers

Problem

Incompressible neo-Hookean hyperelasticity with growth (morphoelasticity)



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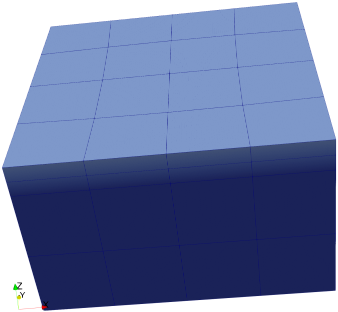

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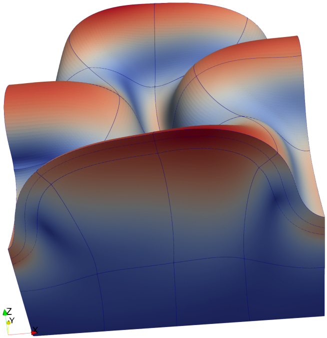

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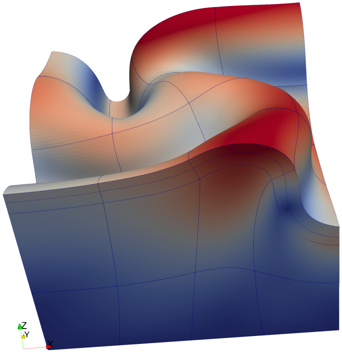

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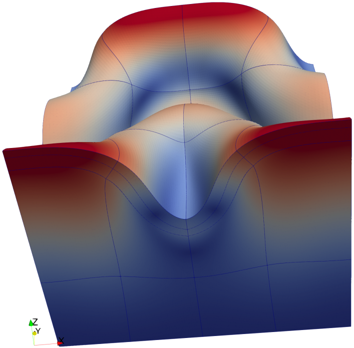

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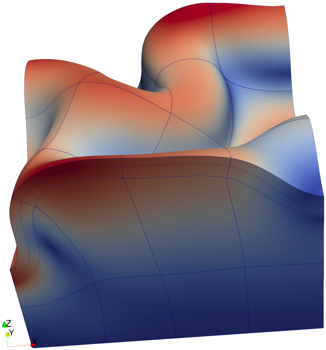

Application: Bose–Einstein condensates

Stationary Gross–Pitaevskii equation

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

Application: Bose–Einstein condensates

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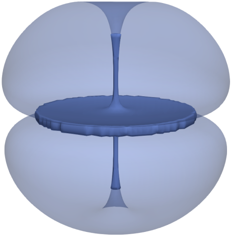

Solutions for $\mu = 6$. A vortex line and a planar dark soliton.

Application: Bose–Einstein condensates

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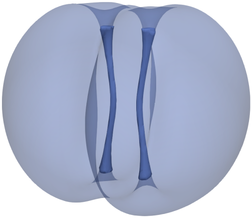

Solutions for $\mu = 6$. A pair of vortex lines.

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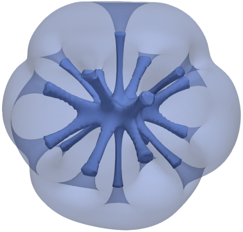

Solutions for $\mu = 6$. A vortex star.

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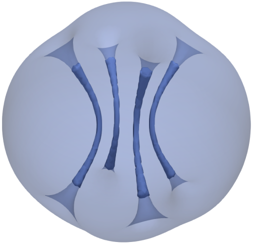
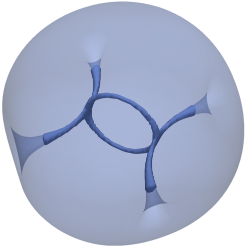


Solutions for $\mu = 6$. Four vortex lines of alternating charge.

Application: Bose–Einstein condensates

Stationary Gross–Pitaevskii equation

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

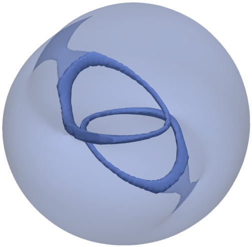


Solutions for $\mu = 6$. A vortex ring with two "handles".

Application: Bose–Einstein condensates

Stationary Gross–Pitaevskii equation

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



Solutions for $\mu = 6$. Two bent vortex rings?

Application: Bose–Einstein condensates

Stationary Gross–Pitaevskii equation

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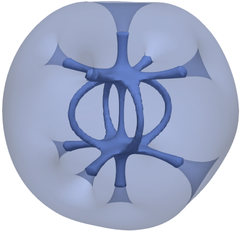
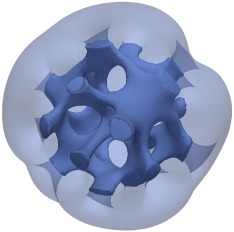


Solutions for $\mu = 6$. Two vortex rings and five lines?

Application: Bose–Einstein condensates

Stationary Gross–Pitaevskii equation

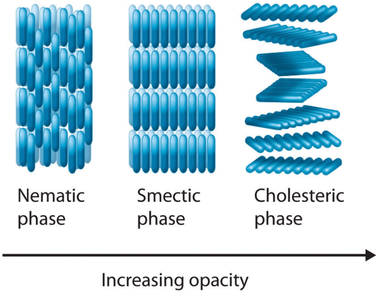
$$-\frac{1}{2}\Delta\phi + \frac{x^2+y^2+z^2}{2}\phi - \mu\phi + |\phi|^2\phi = 0, \qquad \phi|_{\partial\Omega} = 0.$$



Solutions for $\mu = 6$. A vortex ring cage?

Smectic-A liquid crystals

An exotic state of matter with properties between fluids and crystalline solids.



Source: Averill & Eldridge (2011).

Smectic-A liquid crystals

A new model, proposed by Xia, F., et al.:

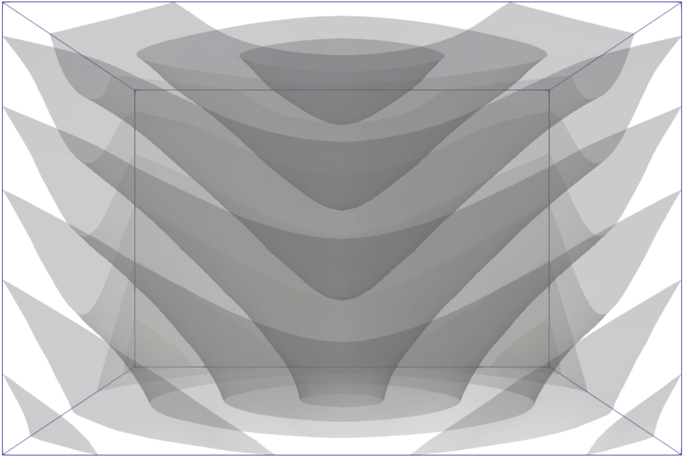
Energy functional for smectic liquid crystals

$$
\begin{aligned}
J(\mathbf{Q}, \delta\rho) = & \int_\Omega \left(\frac{a}{2}(\delta\rho)^2 + \frac{b}{3}(\delta\rho)^3 + \frac{c}{4}(\delta\rho)^4 \right) \\
& + \int_\Omega B \left[D^2 \delta\rho + q^2 (\mathbf{Q} + I/3)\delta\rho \right]^2 \\
& + \int_\Omega \left(\frac{K}{2} |\nabla \mathbf{Q}|^2 - \frac{\ell}{2}(\mathrm{tr}(\mathbf{Q}^2)) - \frac{\ell}{3}(\mathrm{tr}(\mathbf{Q}^3)) + \frac{\ell}{2}(\mathrm{tr}(\mathbf{Q}^2))^2 \right) \\
& + \int_{\text{bottom}} \frac{w}{2} \left(\nu \cdot (\mathbf{Q} + I/3)\nu \right) - \int_{\text{top}} \frac{w}{2} \left(\nu \cdot (\mathbf{Q} + I/3)\nu \right).
\end{aligned}
$$

Here $\mathbf{Q}(x) \in \mathbb{R}^{2\times 2}$ is symmetric and traceless and $\delta\rho(x) \in \mathbb{R}$.

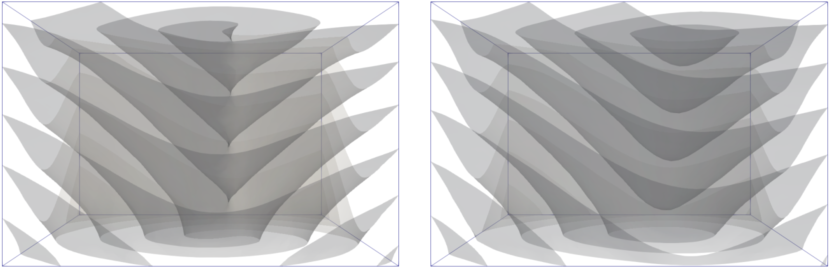
Parameters: $a = -10, b = 0, c = 10, B = 10^{-5}, K = 0.3, q = 30, \ell = 30, w = 3.$

Smectic-A liquid crystals



A toroidal focal conic domain, captured numerically for the first time.

Smectic-A liquid crystals



Two solutions for the same parameter values.

Semismooth equations

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Deflation works for semismooth problems (**variational inequalities**).

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Theorem (F., Surowiec, 2017)

Let $F : V \to V^*$ be a semismooth map between a Banach space and its dual. Let $r \in V$ be a root of F. Suppose r satisfies the assumptions required for superlinear convergence of the semismooth Newton method given in Hintermüller, Ito and Kunisch (2002). Then the operator

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

is a deflation operator for $p \geq 1$.

Buckling of a hyperelastic beam with contact constraints

Neo–Hookean compressible hyperelasticity

$$
\begin{aligned}
\underset{u\in H^1(\Omega;\mathbb{R}^2)}{\text{minimise}} \quad & \Pi(u) = \int_\Omega \psi(u)\ \mathrm{d}x - \int_\Omega B\cdot u\ \mathrm{d}x \\
\text{subject to} \quad & u|_{\text{left}} = (0,0),\ \ u|_{\text{right}} = (-\varepsilon, 0), \\
& \mathrm{tr}(u_y) \in [a,b] \text{ a.e. in } \Gamma_{\text{top}}, \Gamma_{\text{bottom}}.
\end{aligned}
$$

Buckling of a hyperelastic beam with contact constraints

Neo–Hookean compressible hyperelasticity

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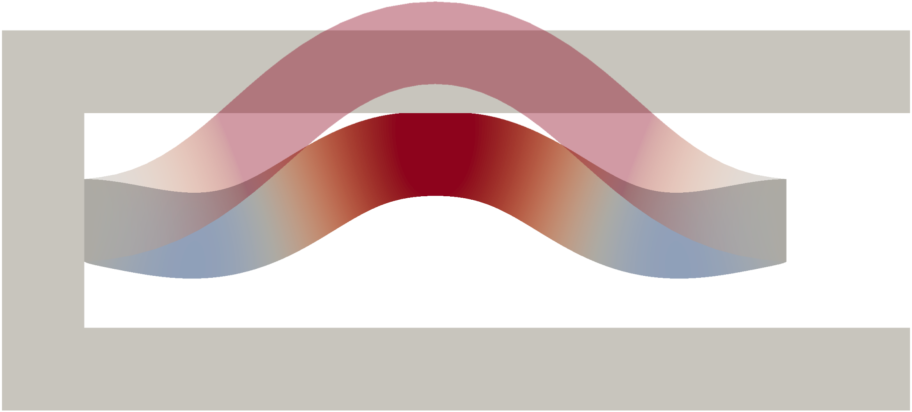
Strain energy density

$$\psi(u) = \frac{\mu}{2}(\mathrm{tr}(C) - 2) - \mu \log(\det(C)) + \frac{\lambda}{2}\log(\det(C))^2,$$

where

$$C = (I + \nabla u)^\top (I + \nabla u).$$

Buckling of a hyperelastic beam with contact constraints



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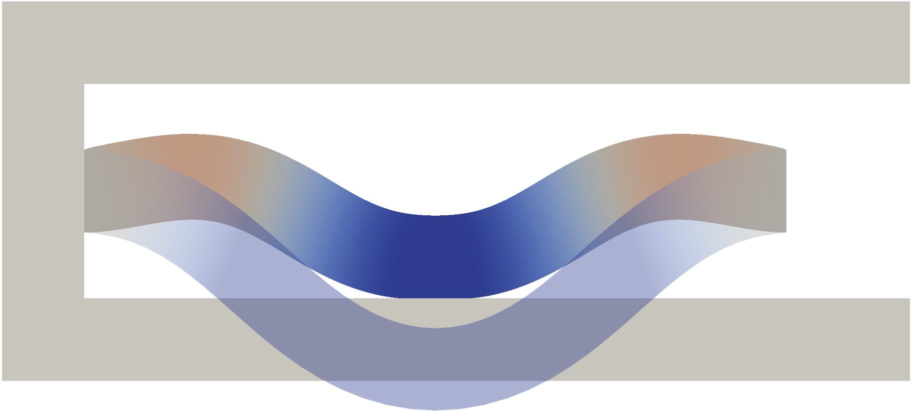

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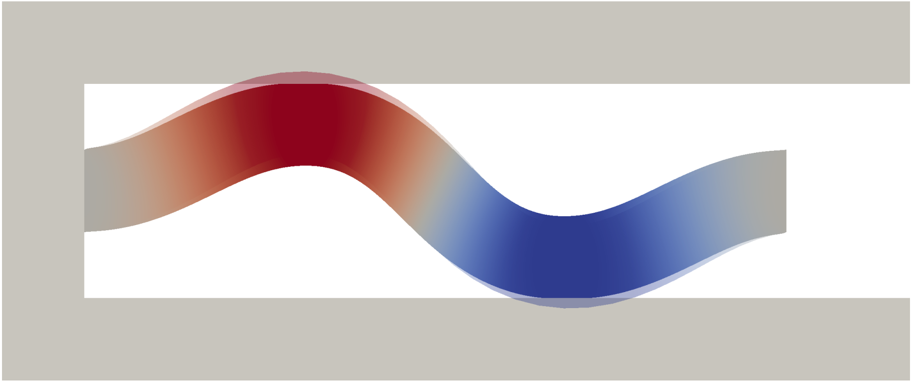

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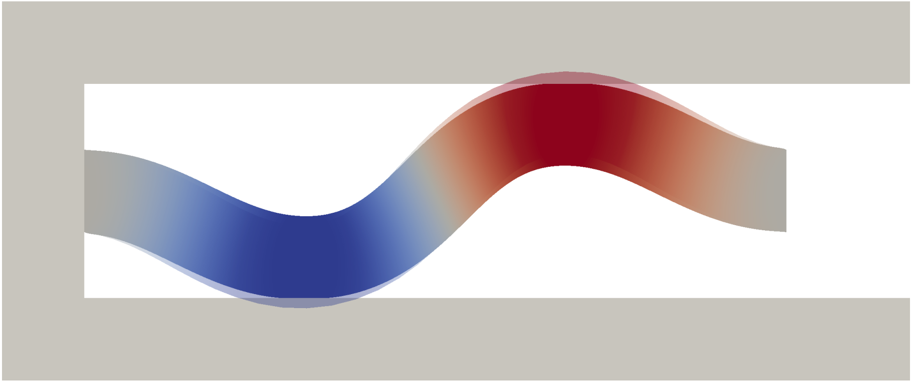

Conclusions

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- Deflation is a useful technique for finding them.
- Deflated problems can be **solved efficiently**.