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?
Can you conduct an experiment twice . . . and get two different answers?

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 $\lambda$. 
Mathematical formulation

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Aircraft stiffener

$u$ displacement, $\lambda$ loading, $f$ hyperelasticity
Mathematical formulation

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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

\[ u \]

\[ \lambda \]
Branch switching

Step I: continuation
Branch switching

Step II: continuation
Branch switching

Step III: detect bifurcation point
Step IV: compute eigenvectors and switch
Branch switching

Step V: continuation on branches
A disconnected diagram.
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 $\lambda$. Given

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

**Deflation**

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

construct a **new nonlinear problem** $\mathcal{G} : V \to V^*$ such that:

- **(Preservation of solutions)** $\mathcal{F}(\tilde{r}) = 0 \iff \mathcal{G}(\tilde{r}) = 0$ for all $\tilde{r} \neq r$
- **(Deflation property)** Newton's method applied to $\mathcal{G}$ will never converge to $r$ again, starting from any initial guess.

Find more solutions, starting from the same initial guess.
The core idea

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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

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

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

Step III: termination on nonconvergence
Finding many solutions from the same guess

Step III: termination on nonconvergence
Construction of deflated problems

A nonlinear transformation

\[ G(u) = M(u; r)F(u) \]
Construction of deflated problems

A nonlinear transformation

\[ G(u) = M(u; r)F(u) \]

A deflation operator

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

\[ \liminf_{u \to r} \| G(u) \|_{V^*} = \liminf_{u \to r} \| M(u; r)F(u) \|_{V^*} > 0 \]
Construction of deflated problems

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

Theorem (F., Birkisson, Funke, 2014)

This is a deflation operator for \( p \geq 1 \):

\[ M(u; r) = \left( \frac{1}{\|u - r\|^p} + 1 \right) \]
Deflated continuation

\[ u \]

\[ \lambda \]
Deflated continuation

Step I: continuation
Deflated continuation

Step II: continuation
Deflated continuation

Step III: deflate

\( \lambda \)

\( u \)
Deflation

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
A disconnected diagram.
Section 4

Computations
A question

How do we solve the deflated problem?
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

\[ J_G(u) \Delta u_G = -G(u) \]
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

\[ J_G(u) = M(u; r) J_F(u) + F(u) M'(u; r)^T \]
A Newton step

\[ J_F(u) \Delta u_F = -F(u) \]

A deflated Newton step

\[ J_G(u) \Delta u_G = -M(u)F(u) \]

Deflated Jacobian

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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 \( M' \).
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

Solutions of $\varepsilon^2 y'' + 2(1 - x^2)y + y^2 - 1 = 0$

Pitchfork bifurcation
Application: Carrier’s problem

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Pitchfork bifurcation
Fold bifurcation
Application: Carrier’s problem

Solutions of $\varepsilon^2 y'' + 2(1 - x^2)y + y^2 - 1 = 0$
Application: Carrier’s problem

Pitchfork bifurcations

\[ \varepsilon \approx \frac{0.472537}{n} \]
Application: Carrier’s problem

Pitchfork bifurcations

\[ \varepsilon \approx \frac{0.472537}{n} \]

<table>
<thead>
<tr>
<th>Connected component</th>
<th>Computed ( \varepsilon )</th>
<th>Asymptotic estimate</th>
<th>Relative error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.46886251</td>
<td>0.472537</td>
<td>0.7837%</td>
</tr>
<tr>
<td>2</td>
<td>0.23472529</td>
<td>0.236269</td>
<td>0.6574%</td>
</tr>
<tr>
<td>3</td>
<td>0.15703946</td>
<td>0.157512</td>
<td>0.3012%</td>
</tr>
<tr>
<td>4</td>
<td>0.11798359</td>
<td>0.118134</td>
<td>0.1278%</td>
</tr>
</tbody>
</table>

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

\[ \varepsilon \approx \frac{0.472537}{n} - \frac{0.8344}{n} \]

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<tbody>
<tr>
<td>2</td>
<td>0.28522538</td>
<td>0.298545</td>
<td>4.670%</td>
</tr>
<tr>
<td>3</td>
<td>0.17186970</td>
<td>0.173608</td>
<td>1.011%</td>
</tr>
<tr>
<td>4</td>
<td>0.12421206</td>
<td>0.124634</td>
<td>0.3397%</td>
</tr>
<tr>
<td>5</td>
<td>0.09762446</td>
<td>0.0977706</td>
<td>0.1497%</td>
</tr>
</tbody>
</table>

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 $V = 1.1$. 

![Graphs showing 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
Applications: 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 $D = 1.5 \, \mu m$. 
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
Application: geometrically frustrated cholesteric

Energy functional vs Cholesteric pitch $q_o$
Application: geometrically frustrated cholesteric
Application: smectic-A

Pevnyi–Selinger–Sluckin (2014) model

Minimise

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

subject to $n \cdot n = 1$, periodic in $x$, Dirichlet on $n$ for $y \in \{0, 1\}$.
Application: smectic-A

Pevnyi–Selinger–Sluckin (2014) model

Minimise

\[ J(n) = \int_{\Omega} \left( \frac{a}{2} \delta \rho^2 + \frac{c}{4} \delta \rho^4 + B \left| \nabla \nabla \delta \rho + q^2 n \otimes n \delta \rho \right|^2 + \frac{K}{2} |\nabla n|^2 \right) \, dx \]

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

Difficult discretisation

Finite element discretisation is difficult because \( \delta \rho \in H^2(\Omega) \).
Application: smectic-A

Pevnyi–Selinger–Sluckin (2014) model

Minimise

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

Difficult discretisation

Finite element discretisation is difficult because \( \delta \rho \in H^2(\Omega) \).

Solution: nonconforming Morley element
Application: smectic-A

\[ \delta \rho \] for some of 73 solutions found for \( q = 30, a = -10, c = 10, B = 10^{-5}, K = 0.3. \]
Multiple solutions are **ubiquitous and important** in liquid crystals.
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Deflation is a **useful technique** for finding them.
Conclusions

- Multiple solutions are ubiquitous and important in liquid crystals.
- Deflation is a useful technique for finding them.
- Deflated problems can be solved efficiently.