COMPRESSION OF A HYPERELASTIC BEAM
DEFLATION TECHNIQUES

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Abstract. The aim of this text is to reproduce the bifurcation diagram of an example from the Defcon package, namely compression of a hyperelastic beam, using own implementation of the deflation techniques in FEniCS computational platform.

Contents

1. Introduction

Deflation techniques are methods for finding distinct solutions of stationary nonlinear equations. For further discussion, see Farrell et al. (2015) and Farrell et al. (2016). From recent works we can mention Xia et al. (2020) and Boullé et al. (2022).

Let us suppose a nonlinear problem with parameter λ and unknown u:

$$F(u, \lambda) = 0.$$

According to the parameter λ, the problem can have several distinct solutions. Further suppose, we know k solutions u_r at one specific λ where k is less than number of all existing solutions. The essence of the deflation technique is to suppress the Newton convergence to known k solutions u_r in order to look for another solution. We construct the so-called deflation problem:

$$M(u, u_r)F(u, \lambda) = 0$$

with the deflation operator in the form:

$$M(u, u_r) = \prod_{r=1}^{k} \left(\frac{1}{||u - u_r||^p} + \alpha \right).$$

The properties of deflation and deflation operator are discussed in Farrell et al. (2015). We try to find as many solutions as possible for the fixed λ. Then by continuation step we proceed to new value of λ.

Many sophisticated methods can be used for the continuation, for example tangent (secant) or arclength (pseudoarclenght) continuation, see Allgower and Georg (2003). In our case, we use the classical continuation, when the found solutions at λ is used as initial guesses for the Newton method at $\lambda + \Delta\lambda$.

In this text, we compare two possible implementations of the deflation techniques and compare them in solving a physical problem, compression of a hyperelastic beam, discussed in Section 2. The first implementation is based on the Sherman-Morison formula, see Section 3. The second one is based on the Lagrange multipliers, see Section 4.

We investigate two benchmarks, the full construction of a bifurcation diagram (Section 5) and how many different solutions we can find by deflation from the main branch, see Section 6. The bifurcation diagrams can be also compared to diagrams obtained by the Defcon package[1].

2. Problem

This specific problem is solved in Farrell et al. (2016). The implementation can be found in the Defcon package[2].

Consider a two-dimensional hyperelastic beam with length 1.0 m and width 0.1 m. We denote the domain by $\Omega = (0, 1) \times (0, 0.1)$. The left face of the beam is fixed, and constant displacement $u = (-\lambda, 0)$ is prescribed on the right (λ is the parameter determining number of solutions). The other lateral faces are traction free. In order to break a symmetry

[1] `https://bitbucket.org/pefarrell/defcon`

[2] `https://bitbucket.org/pefarrell/defcon/src/master/examples/fenics/hyperelasticity/hyperelasticity.py`

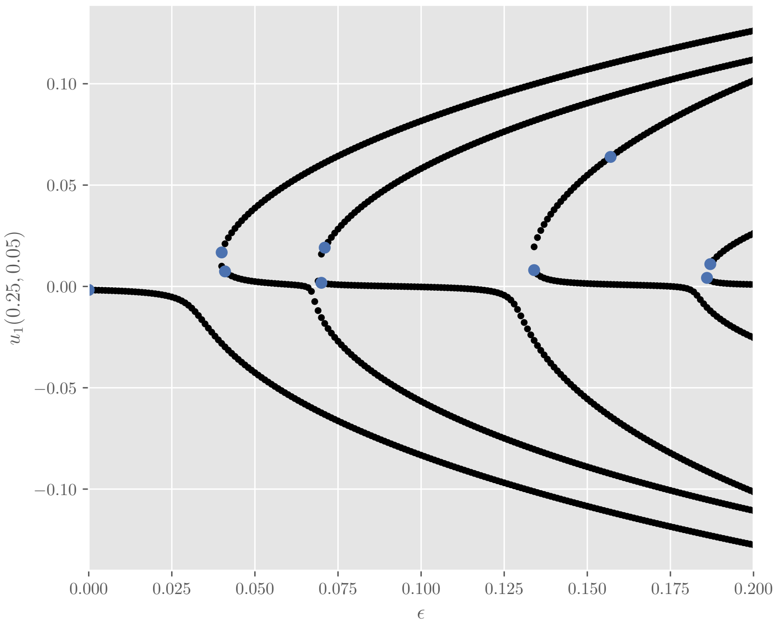


FIGURE 1. Bifurcation diagram by the Defcon package

of solutions, we prescribe also a body force $b = (0, -1000)$. The beam is compressible neo-Hookean hyperelastic material described by the strain energy density function:

$$W(u) = \frac{\mu}{2}\left(|\mathbb{F}|^2 - 2\right) - \mu \ln(\det \mathbb{F}) + \frac{\lambda}{2}\ln^2(\det \mathbb{F})$$

where $\mathbb{F} = \mathbb{I} + \operatorname{grad} u$ and Lamé parameters $\mu = \frac{\mathrm{E}}{2(1+\nu)}$, $\lambda = \frac{\mathrm{E}\nu}{(1+\nu)(1-2\nu)}$. We choose material parameters as:

$$\mathrm{E} = 1000000.0,$$
$$\nu = 0.3.$$

The problem is to minimalise the functional in the form:

$$\min_{\substack{u \\ u(0,\cdot)=(0,0) \\ u(1,\cdot)=(-\lambda,0)}} \int_\Omega W(u) - b \cdot u \; \mathrm{d}v.$$

The number of solutions depends on the parameter λ, see Figure 4. The bifurcation diagrams captures the behavioural of a chosen functional of the solutions as λ varies. We choose two functionals: the total energy:

$$E = \int_\Omega W(u) \; \mathrm{d}v$$

and the displacement $u^x(0.25, 0.05)$. The bifurcation diagram obtained by the Defcon package is shown in Figure 1. We can see, that the maximum number of solutions is nine in interval of interest $\lambda \in [0.0, 0.2]$. We note that the branches are disconnected. They are series of fold bifurcations and they can be viewed as a perturbation of the pitchfork bifurcations for the problem without body force (symmetrical case).

3. Implementation - Sherman–Morrison formula

Consider a non-linear problem which takes the form:

$$F(u, \lambda) = 0. \tag{1}$$

In our case, we deal with the system $\boldsymbol{F}$ which comes from the discretization of the weak formulation using the finite element method. To solve the equations for a fix parameter λ, we use the Newton method:

$$\boldsymbol{u}_{n+1} = \boldsymbol{u}_n + \boldsymbol{\delta}_F,$$
$$\mathbb{J}_F(\boldsymbol{u}_n)\boldsymbol{\delta}_F = -\boldsymbol{F}(\boldsymbol{u}_n),$$

where $\boldsymbol{u}_n$ is the nth iteration vector containing degrees of freedom, $\boldsymbol{\delta}_F$ is the Newton step and $\mathbb{J}_F = \frac{\partial \boldsymbol{F}}{\partial \boldsymbol{u}}$ is the Jacobian matrix.

Assume, we know k solutions u_r of the problem (1). In the aim to find another solution, we define the so-called deflated operator $M(u, u_r)$:

$$M(u,u_r) = \prod_{r=1}^{k}\left(\frac{1}{\|u-u_r\|^p}+\alpha\right)$$

and the deflated problem:

$$M(u,u_r)F(u,\lambda) = 0, \tag{2}$$

where p is a power, α is a shift and $\|\cdot\|$ is a convenient norm. By the same discretization process, we obtain the Newton iterations in the form:

$$\begin{aligned}\boldsymbol{u}_{n+1} &= \boldsymbol{u}_n + \boldsymbol{\delta}_D,\\ \mathbb{J}_D(\boldsymbol{u}_n)\boldsymbol{\delta}_D &= -M(\boldsymbol{u}_n,\boldsymbol{u}_r)\boldsymbol{F}(\boldsymbol{u}_n).\end{aligned}$$

Now, the Jacobian matrix $\mathbb{J}_D$ is rank-one permutation of the original Jacobian matrix $\mathbb{J}_F$ and M is scalar:

$$\mathbb{J}_D = M(\boldsymbol{u}_n,\boldsymbol{u}_{r_n})\mathbb{J}_F + \boldsymbol{F}(\boldsymbol{u}_n)\otimes\boldsymbol{d}(\boldsymbol{u}_n,\boldsymbol{u}_r),$$

where we denote $\boldsymbol{d} = \frac{\partial M}{\partial \boldsymbol{u}}$.

The key idea of implementation is to find relation between the Newton steps $\boldsymbol{\delta}_D$ and $\boldsymbol{\delta}_F$ and use the information about $\mathbb{J}_F$. In what follows, we omit arguments in our notation for brevity. We start with:

$$\boldsymbol{\delta}_D = -\mathbb{J}_D^{-1}(M\boldsymbol{F}) = \mathbb{J}_D^{-1}(M\mathbb{J}_F\boldsymbol{\delta}_F). \tag{3}$$

To compute the inverse of $\mathbb{J}_D$, we use the Sherman–Morrison formula 3.1:

$$\mathbb{J}_D^{-1} = (M\mathbb{J}_F + \boldsymbol{F}\otimes\boldsymbol{d})^{-1} = (M\mathbb{J}_F)^{-1} - \frac{(M\mathbb{J}_F)^{-1}\boldsymbol{F}\boldsymbol{d}^\intercal(M\mathbb{J}_F)^{-1}}{1+\boldsymbol{d}^\intercal(M\mathbb{J}_F)^{-1}\boldsymbol{F}}.$$

We substitute this into (3) and use $\mathbb{J}_F\boldsymbol{\delta}_F = -\boldsymbol{F}$:

$$\begin{aligned}\boldsymbol{\delta}_D &= \left(\mathbb{I} - \frac{(M\mathbb{J}_F)^{-1}\boldsymbol{F}\boldsymbol{d}^\intercal}{1+\boldsymbol{d}^\intercal(M\mathbb{J}_F)^{-1}\boldsymbol{F}}\right)\boldsymbol{\delta}_F,\\ \boldsymbol{\delta}_D &= \left(\mathbb{I} - \frac{M^{-1}\boldsymbol{d}^\intercal\boldsymbol{\delta}_F}{1+M^{-1}\boldsymbol{d}^\intercal\boldsymbol{\delta}_F}\right)\boldsymbol{\delta}_F.\\ \boldsymbol{\delta}_D &= \frac{\boldsymbol{\delta}_F}{1-M^{-1}\boldsymbol{d}^\intercal\boldsymbol{\delta}_F}.\end{aligned}$$

In summary, the deflated problems can be solved by the Newton method as the original problems, only at each step the Newton iteration is modified as:

$$\boldsymbol{\delta}_D = \frac{\boldsymbol{\delta}_F}{1-M^{-1}\boldsymbol{d}\cdot\boldsymbol{\delta}_F}. \tag{4}$$

Together, we get:

$$\begin{aligned}\boldsymbol{u}_{n+1} &= \boldsymbol{u}_n + \boldsymbol{\delta}_D,\\ \boldsymbol{\delta}_D &= \frac{\boldsymbol{\delta}_F}{1-M^{-1}\boldsymbol{d}\cdot\boldsymbol{\delta}_F}\\ \mathbb{J}_F(\boldsymbol{u}_n)\boldsymbol{\delta}_F &= -\boldsymbol{F}(\boldsymbol{u}_n).\end{aligned}$$

Lemma 3.1 (Sherman–Morrison formula)**.** *Let $\mathbb{A}$ be an invertible matrix, $\boldsymbol{u}$ and $\boldsymbol{v}$ arbitrary vectors. Suppose that $\boldsymbol{v}\cdot\mathbb{A}^{-1}\boldsymbol{u} \neq -1$. Then:*

$$(\mathbb{A}+\boldsymbol{u}\otimes\boldsymbol{v})^{-1} = \mathbb{A}^{-1} - \frac{1}{1+\boldsymbol{v}\cdot\mathbb{A}^{-1}\boldsymbol{u}}(\mathbb{A}^{-1}\boldsymbol{u})\otimes(\mathbb{A}^{-\intercal}\boldsymbol{v})$$

4. Implementation - Lagrange multipliers

Suppose, we have the deflated problem (2) as in Section 3. We introduce k Lagrange multipliers p_r as:

$$\underbrace{\left(\frac{1}{\|u-u_k\|^p}+\alpha\right)}_{p_k}\cdots\underbrace{\left(\frac{1}{\|u-u_2\|^p}+\alpha\right)}_{p_2}\underbrace{\left(\frac{1}{\|u-u_1\|^p}+\alpha\right)}_{p_1}F(u,\lambda) = 0.$$

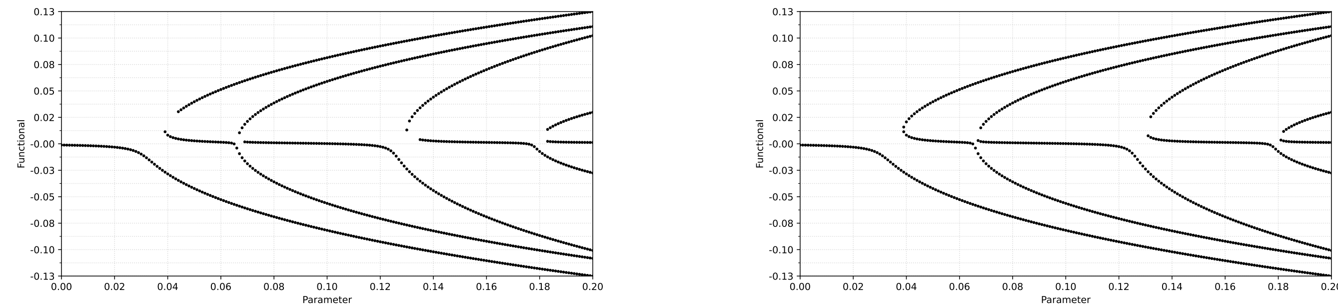
By simple manipulation, we obtain an equation for p_r:

$$\|u-u_r\|^p\,(p_r-\alpha) = 1.$$

We multiply this equation by test scalar $\tilde{p}$ and integrate it over the domain Ω:

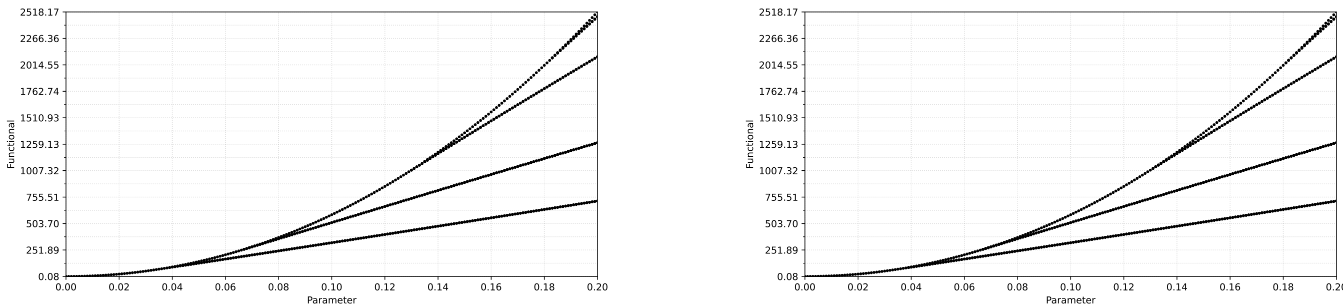
$$\int_\Omega \tilde{p}\|u-u_r\|^p\,(p_r-\alpha) - \tilde{p}\;\mathrm{d}v.$$

Then this k additional equations are added to the original system (1).



(A) Lagrange multipliers (B) Sherman–Morrison formula

Figure 2. Bifurcation diagrams by naive implementations for displacement $u^x(0.25, 0.05)$



(A) Lagrange multipliers (B) Sherman–Morrison formula

Figure 3. Bifurcation diagrams by naive implementations for total energy

An initial guess of p is required for the Newton method. In our computation, we start with $p = 100000$. This number was chosen by experiments.

5. Bifurcation diagrams

Our naive implementation of the deflated continuation between values $[\lambda_{\text{start}}, \lambda_{\text{end}}]$, see Farrell et al. (2016), consists of several steps:

- find a solution at λ_{start} using initial guess $u_0 = (0, 0)$,
- find the main branch $[\lambda_{\text{start}}, \lambda_{\text{end}}]$ by classical continuation,
- repeat the cycle with λ until $\lambda = \lambda_{\text{end}}$
  - do deflation from all known branches, as initial guess use previous solution at the deflated branch, try to find as many solutions as possible,
  - once new solution or solutions are found, proceed with classical continuation (initial guess is the solution at λ in the specific branch) to the end, i.e. $(\lambda, \lambda_{\text{end}}]$
  - continue with new value $\lambda + \Delta\lambda$, where $\Delta\lambda$ is sufficiently small.

Note that we use only continuation forwards and unlike the Defcon package, our naive implementation is purely sequential. Our results, see Figures 2 and 3, are comparable with the results obtained by the Defcon package, see Figure 1.

6. Deflation from the main branch

We ask a question, how many successful deflations can be obtained when we deflate the main branch, depending on considered mesh or used implementation. We compute several diagrams with different settings, see Table 1. Results are shown in Figures 5. If we compare the diagrams, we can see that there are clusters where implementation based on Sherman-Morrison converged and the implementation based on Lagrange multipliers not and vice-versa. Number of successful deflations does not have to be bigger with a refined mesh. We can conclude that the deflation techniques depend on considered settings.

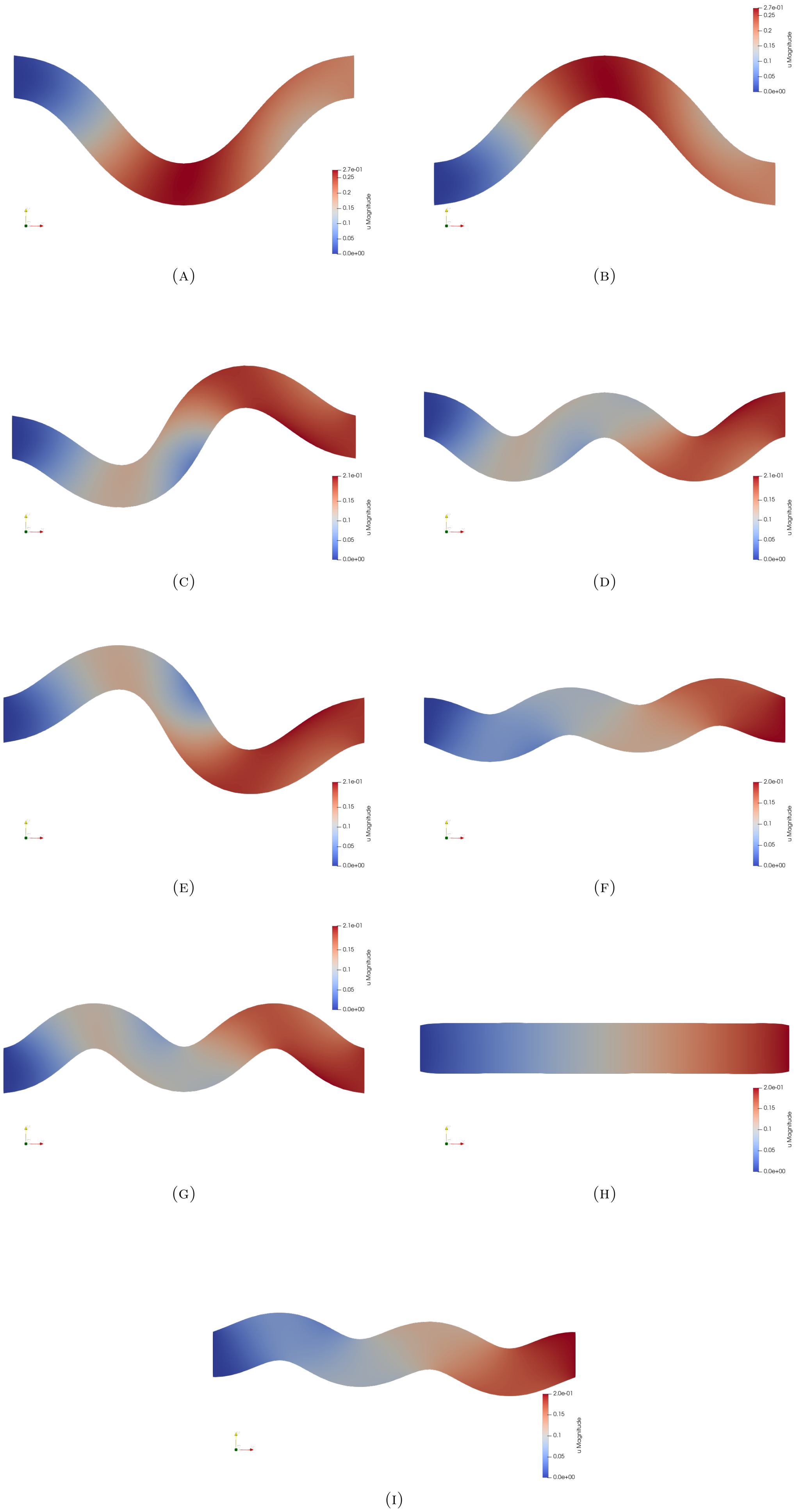
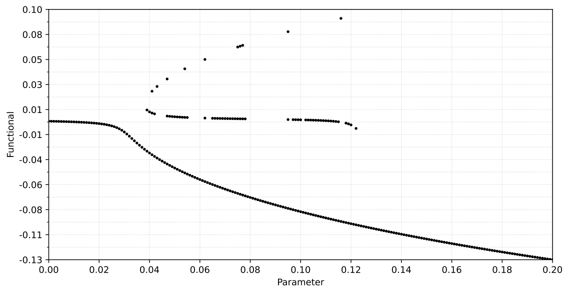
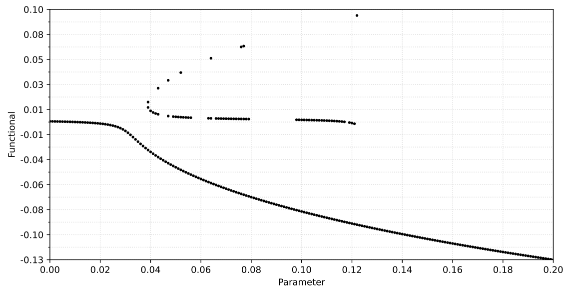


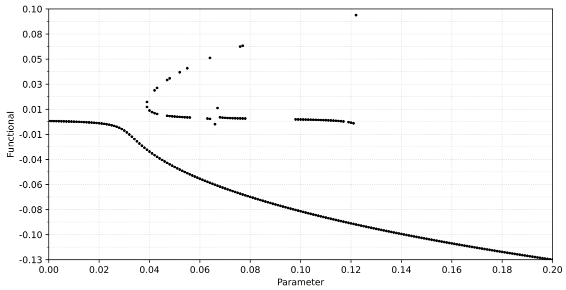
FIGURE 4. Nine solutions for parameter $\lambda = 0.198$



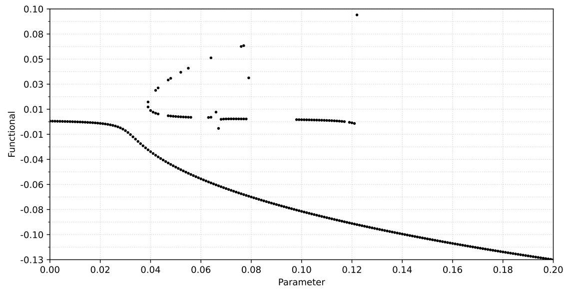
(A)



(B)



(C)



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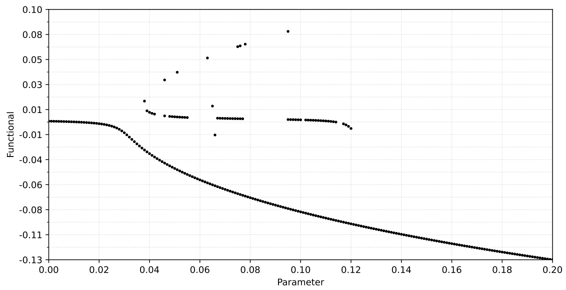

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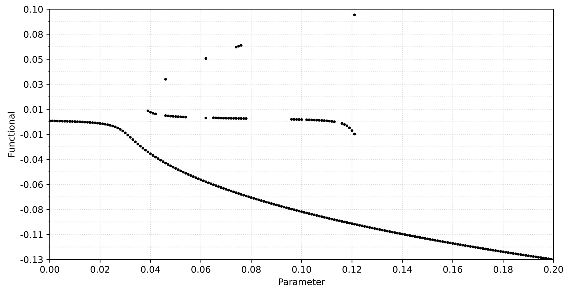

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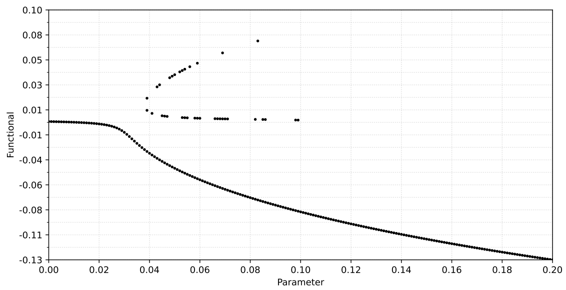
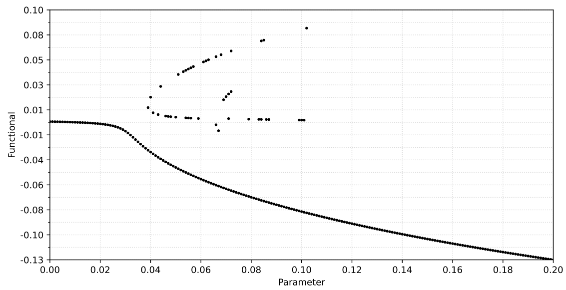
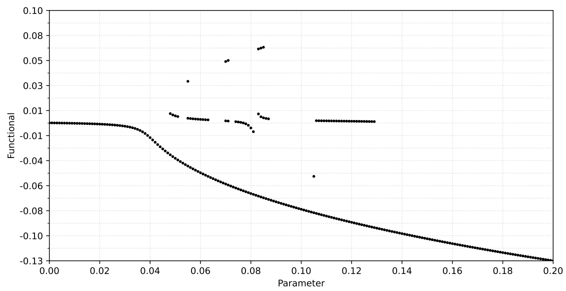


(G)



(H)



(I)

FIGURE 5. Deflation from the main branch, settings in Table 1.

Test	Implementation	Mesh type	Elements	d
A	Sherman	crossed	(50, 50)	61
B	Sherman	right/left	(50, 50)	61
C	Sherman	right	(50, 50)	64
D	Sherman	left	(50, 50)	65
E	Sherman	right	(100, 100)	57
F	Sherman	right	(150, 150)	57
G	Lagrange	crossed	(50, 50)	35
H	Lagrange	right	(50, 50)	43
I	Sherman	right	(20, 20)	59

Table 1. Parameters for all tests, number d is number of sucessful deflations.

7. Attachments

List of enclosed scripts:

(1) `hyperelasticity.py`, example from the Defcon package,
(2) `Problem.py`, main script to construct bifurcation diagrams,
(3) `Problem_one_branch.py`, deflation from the main branch,
(4) `Deflated_Newton.py`, explicit implementation of the Newton method and modification of the Newton method to solve the deflated problems (Sherman–Morrison and Lagrange multipliers),
(5) `save_read.py`, to save or read solutions in `h5` files,
(6) `save_xdmf.py`, to save `xdmf` files.

References

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Boullé, N., V. Dallas, and P. E. Farrell (2022, May). Bifurcation analysis of two-dimensional rayleigh-bénard convection using deflation. *Phys. Rev. E 105*, 055106.

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