Optimal management and spatial patterns in a distributed shallow lake model

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Abstract

We present a framework to numerically treat spatially distributed optimal control problems with an infinite time horizon. The basic idea is to consider the associated canonical system in two steps. First we perform a bifurcation analysis of the steady state canonical system using the continuation and bifurcation package \texttt{pde2path}, yielding a number of so called flat and patterned canonical steady states. In a second step we link \texttt{pde2path} to the two point boundary value problem solver \texttt{TOM} to study time dependent canonical system paths to steady states having the so called saddle point property. As an example we consider a shallow lake model with diffusion.

1 Introduction

In [BX08] the authors consider deterministic optimal control (OC) problems with a continuum of spatial sites over which the state variable can diffuse. They derive the remarkable result that under certain conditions on the Hamiltonian for the optimally controlled system there occurs a Turing like bifurcation of steady states of the canonical system, and call this phenomenon optimal diffusion-induced instability (ODI). Here we present a numerical framework to (a) study such ODI bifurcations of canonical steady states (CSS) numerically in a simple way, and (b) study their optimality by calculating and evaluating time–dependent paths to and from such CSS. As an example we use one of the three examples presented in [BX08], namely a version of the, in the field of ecological economics, well-known shallow lake optimal control (SLOC) model, cf. [Sch98, MXdZ03, CB04].

We use the acronyms FCSS and PCSS for flat and patterned canonical steady states, and similarly FOSS and POSS for optimal canonical steady states, and summarize FOSS and POSS as OSS. The SLOC model has up to three (branches of) FCSS in relevant parameter regimes, and in these regimes we also find a large number of (branches of) PCSS. In this situation of multiple CSS a local stability analysis at a given CSS is in general not sufficient. Here, local stability analysis means that the stationary canonical system is analyzed, analogous to a steady-state analysis of the canonical system derived from an optimal control problem without spatial diffusion. It is well known and shown for many models that the appearance of multiple steady-states in the canonical system (even if these steady-states are saddle-points) does not necessarily imply the appearance of multiple steady-states in the optimal system, cf. [GCF+08, KW10]. The reason is that there can exist a non–constant extremal solution, i.e. a trajectory that satisfies the necessary optimality conditions, connecting the state values of the steady-state in consideration to some other state, and yielding a higher objective value. Therefore, to study whether a CSS corresponds to an OSS, the values on the associated stable paths also have to be considered, which requires an efficient numerical algorithm.

Thus, here we calculate the bifurcation behavior of FCSS and PCSS for the SLOC model in some detail, and study their optimality by evaluation of their objective functions $J$ and comparison to...
time-dependent canonical paths. Such a global analysis is inevitable and has to accompany the local stability analysis. Since in general the pertinent ODEs or PDEs cannot be solved analytically we have to use numerical methods for the calculation of FCSS and in particular PCSS, and for the calculation of the corresponding $t$–dependent canonical paths. For the steady state problem we use the continuation and bifurcation software \texttt{pde2path}, which we then simply combine with the boundary value problem (BVP) solver TOM to obtain canonical paths.\footnote{Our software, including demo files and a manual to run some of the simulations in this paper, can be downloaded from \url{www.staff.uni-oldenburg.de/hannes.uecker/pde2path}.}

In the remainder of this introduction we present the SLOC model with and without diffusion, give the associated canonical systems, and in particular discuss the asymptotic transversality condition and the saddle point property (SPP) used to convert the SLOC model from an infinite time horizon to a numerically treatable BVP in $t$. In §2 we explain the numerics to first calculate the bifurcation diagram for the stationary canonical system, and then to solve the $t$ BVP, and explain our main results. We mostly focus on one spatial dimension (1D), but also give a short outlook on the 2D case.

Clearly, our method can be applied to a large variety of similar spatially distributed OC problems, and some studies of such problems are underway. A summary, and plans for extensions, are given in the discussion in §3.

1.1 The shallow lake model without diffusion

A well known non–distributed or 0D version of the SLOC model, see e.g. [Wag03], can be formulated in dimensionless form as

$$V(P_0) := \max_{k(\cdot)} J(P_0, k(\cdot)), \quad J(P_0, k(\cdot)) := \int_0^{\infty} e^{-rt} J_c(P(t), k(t)) \, dt,$$  \hspace{1cm} (1a)

where $J_c(P, k) = \ln(k) - \gamma P^2$  \hspace{1cm} (1b)
is the current value objective function, and $P$ fulfills the ODE initial value problem

$$\ddot{P}(t) = k(t) - bP(t) + \frac{P(t)^2}{1 + P(t)^2}, \quad P(0) = P_0 \geq 0.$$  \hspace{1cm} (1c)

Here $r, \gamma, b > 0$ are parameters, $P = P(t)$ is the phosphor contamination of the lake, which we want to keep low for ecological reasons, and $k = k(t)$ is the phosphate load, for instance from fertilizers used by farmers, which farmers want high for economic reasons. The objective function thus consists of the concave increasing function $\ln(k)$, and the concave decreasing function $-\gamma P^2$; $r$ is the discount rate, and $b$ is the phosphor degradation rate in the lake. We consider two scenarios, namely

Scenario 1: $r = 0.03, \gamma = 0.5, b \in (0.5, 0.8)$ (primary bif. param.), \hspace{1cm} (2)

Scenario 2: $r = 0.3, b = 0.55, \gamma \in (2.5, 3.7)$ (primary bif. param.), \hspace{1cm} (3)

and for the distributed case we shall additionally fix the diffusion parameter to $D = 0.5$.

Using Pontryagin’s Maximum Principle an optimal solution $(P^*(\cdot), k^*(\cdot))$ has to satisfy the following optimality conditions, cf. [PBGM62, AK07]:

$$k^*(t) = \arg\max_k H(P^*(t), k, q(t), q_0) \quad \text{for almost all} \quad t \geq 0$$  \hspace{1cm} (4a)

with the Hamiltonian function

$$H(P, k, \lambda, \lambda_0) := q_0 J_c(P, k) + q \left( k - bP + \frac{P^2}{1 + P^2} \right).$$  \hspace{1cm} (4b)
The state \( P^* (\cdot) \) and costate \( q(\cdot) \) paths are solutions of the canonical system\(^2\)

\[
\dot{P}(t) = H_q(P(t),k^*(t),q(t)) = k^*(t) - bP(t) + \frac{P(t)^2}{1 + P(t)^2}, \\
\dot{q}(t) = rq(t) - H_P(P(t),k^*(t),q(t)) = 2\gamma P(t) + q(t) \left( r + b - \frac{2P(t)}{(1 + P(t)^2)^2} \right),
\]

with

\[ P(0) = P_0 > 0, \]

additionaly satisfying the transversality condition

\[ \lim_{t \to \infty} e^{-rt} q(t) = 0 \quad \text{if} \quad \lim_{t \to \infty} P^*(t) > 0. \]  

A solution \((P(\cdot), q(\cdot))\) of the canonical system (5) is called a canonical path, and an equilibrium of (5) is called canonical steady state (CSS). Due to the strict concavity and continuous differentiability of the Hamiltonian function with respect to the control \( k \) the solution of (4a) is given by

\[
\frac{d}{dk} H(P^*(t),k^*(t),q(t)) = 0 \quad \text{which is equivalent to} \quad k^*(t) = -\frac{1}{q(t)}. 
\]

Consequently, for \((P(\cdot), q(\cdot))\) a canonical path, i.e., a solution of the canonical system, with a slight abuse of notation we also call \((P, k)\) with \( k = -1/q \) a canonical path. In particular, if \((\hat{P}, \hat{q})\) is a CSS, so is \((\hat{P}, \hat{k})\). Canonical paths yield candidates for optimal solutions, defined as follows:

**Definition 1.1.** \((P^*(\cdot), k^*(\cdot), P_0)\) is called an optimal solution of (1) if for every admissible \( k(\cdot) \) and associated \( P(\cdot) \) we have

\[
J(P_0, k(\cdot)) \leq J(P_0, k^*(\cdot), P_0) = V(P_0).
\]

Then \( k^*(\cdot, P_0) \) is called an optimal control, \( P^*(\cdot) \) the corresponding optimal (state) path, and

\[
\dot{P}(t) = k^*(t, P_0) - bP(t) + \frac{P(t)^2}{1 + P(t)^2}
\]

is called the optimal ODE. A constant solution \((P^*(\cdot), k^*(\cdot), P_0)\) \((\hat{P}, \hat{k}(\hat{P}))\) of (8) is called an optimal steady state (OSS).

**Remark 1.2.**

(a) Since (1) is autonomous, so is (8), cf. [Wag03]. Specifically \( k^*(t, P_0) \) can be written as a function \( \hat{k}(P(t)) \), which justifies the usage of the term optimal steady state and the usual stability definition in the sense of dynamical systems.

(b) An optimal control \( k^*(\cdot) \) of (1) can be taken as continuous. Hence, for given \( P_0 \) the IVP of (8) has a unique solution. Multiple optimal solutions for given \( P_0 \) can appear since the optimal controls may be different.

(c) A solution path of (5) identifies candidates for optimal solutions, that however need not be optimal.

The long-run behavior of an optimal solution \((P^*(\cdot), k^*(\cdot))\) is described by the following proposition. For a proof see [Wag03, App. A].

\(^2\)It can be proved that the problem is normal, i.e. \( q_0 > 0 \), and hence w.l.o.g. \( q_0 = 1 \) can be assumed and is therefore subsequently omitted.
Proposition 1. If \((P^*(\cdot), k^*(\cdot))\) is an optimal solution of (1), then
\[
\lim_{t \to \infty} (P^*(t), k^*(t)) = (\hat{P}, \hat{k}), \quad \text{with} \quad \hat{k} > 0,
\]
where \((\hat{P}, \hat{k})\) is an OSS.

Proposition 2.

(a) If (5) has a unique CSS \((\hat{P}, \hat{q})\), then \((\hat{P}, \hat{k})\) with \(\hat{k} = -\frac{1}{\hat{q}}\) is an OSS.

In the following, let three distinct CSS exist, where \((\hat{P}, \hat{k})_1\) and \((\hat{P}, \hat{k})_3\) are saddle points.

(a) \((\hat{P}, \hat{k})_1\) is the unique OSS iff for \(P_1(0) = \hat{P}_3\) there exists a path \((P_1(\cdot), q_1(\cdot))\) satisfying (5) and
\[
\lim_{t \to \infty} (P_1(t), q_1(t)) = (\hat{P}_1, \hat{q}_1).
\]

In this case \(\hat{P}_1\) is a globally stable steady state of (8).

(b) Let \((\hat{P}, \hat{k})_2\) be an unstable focus. Then \((\hat{P}, \hat{k})_1\) and \((\hat{P}, \hat{k})_3\) are OSS (w.l.o.g. \(\hat{P}_1 < \hat{P}_3\)) iff there exists a \(P_i\) with \(\hat{P}_1 < P_i < \hat{P}_3\) and paths \((P_i(\cdot), q_i(\cdot))\), \(i = 1, 3\) satisfying (5) and \(P_i(0) = P_i\) with
\[
\lim_{t \to \infty} (P_i(t), q_i(t)) = (\hat{P}_i, \hat{q}_i), \quad \text{and} \quad H(P_i, k_i(0), q_i(0)) = H(P_i, k_3(0), q_3(0)).
\]

Then \(\hat{P}_i, i = 1, 3\) are locally stable steady states of (8).

(c) Let \((\hat{P}, \hat{q})_2\) be an unstable node. Then \((\hat{P}, \hat{q})_1\) and \((\hat{P}, \hat{q})_3\) are OSS (w.l.o.g. \(\hat{P}_1 < \hat{P}_3\)) iff one of the following two cases applies

- There exists a \(P_i\) satisfying the conditions of (b).
- For every \(\varepsilon > 0\) there exist \(\hat{P}_2 - \varepsilon < P_{\varepsilon,1} < P_2 < P_{\varepsilon,2} < \hat{P}_2 + \varepsilon\) and \((P_{\varepsilon}(\cdot), q_{\varepsilon}(\cdot))\), \(i = 1, 3\) satisfying (5) and \(P_{\varepsilon,1}(0) = P_{\varepsilon,1}\) and \(P_{\varepsilon,3}(0) = P_{\varepsilon,2}\) with
\[
\lim_{t \to \infty} (P_{\varepsilon,i}(t), q_{\varepsilon,i}(t)) = (\hat{P}_i, \hat{q}_i) \quad \text{and} \quad \lim_{\varepsilon \to 0} H(P_{\varepsilon,i}, k_{\varepsilon,i}(0), q_{\varepsilon,i}(0)) = H(\hat{P}_2, \hat{K}_2, 2q_2), \quad i = 1, 3.
\]

Then \(P_i, i = 1, 3\) are locally stable steady states and \(\hat{P}_2\) is an unstable steady state of (8).

The proofs follow from the results presented in [KW10, Kis11].

Setting \(u := (P, q)\) and letting \(\check{u}\) be a steady state of (5), the problem is therefore to find a path with \(P(0) = P_0\) and \(\lim_{t \to \infty} u(t) = \check{u}\). To solve this problem numerically different procedures are possible, cf. [LK80]. One approach is to treat (5) on a finite time interval \([0, T]\) and to require \(u(T) \in W_s(\check{u})\), where \(W_s(\check{u})\) is the local stable manifold of \(\check{u}\). In practice we approximate \(W_s(\check{u})\) by the stable eigenspace \(E_s(\check{u})\) and thus require
\[
\bigcup_{\varepsilon > 0} E_s(\varepsilon) = E_s(\check{u}) \quad \text{and} \quad \lim_{t \to \infty} u(t) = \check{u}.
\]

To obtain a well defined two point boundary value problem we then need \(\dim E_s(\check{u}) = 1\).

More generally, if the state variable is an \(n\)-dimensional vector and thus (5) is a system of \(2n\) ODEs, for arbitrary \(P_0\) we need that \(\check{u}\) has the saddle point property, defined as follows.
Definition 1.3 (Saddle Point Property). A CSS $\hat{u} \in \mathbb{R}^{2n}$ with

$$\dim E_s(\hat{u}) = n$$

is called a CSS with saddle point property (SPP). For a CSS having the SPP we also write CSS$^0$. Otherwise we write CSS$^-$. The number

$$d(\hat{u}) := n_s - n$$

is called the defect of $\hat{u}$, and a CSS with defect $\hat{u} < 0$ is called defective.

In [BS76, Roc76, CS76] it is proved that the local stability of an OSS implies the SPP of the according CSS, while already in the classical papers [Kur68b, Kur68a, LS69] about economic growth it has been shown that in case of multiple OSS the according CSS need not satisfy the SPP. In the recent literature such steady states are sometimes called weak Skiba points, cf. [CFJ+05, CFG+13], and in [KW10] the term threshold point is introduced.

1.2 The shallow lake model with diffusion

We consider the shallow lake model with diffusion presented in [BX08], in a domain $\Omega \subset \mathbb{R}^d$, i.e.,

$$V(P_0(\cdot)) := \max_{k(\cdot)} J(P_0(\cdot), k(\cdot, \cdot)), \quad J(P_0(\cdot), k(\cdot, \cdot)) := \int_0^\infty e^{-\gamma t} J_{c,i}(P(t), k(t)) \, dt$$

where $J_{c,i}(P(\cdot, t), k(\cdot, t)) = \int_{\Omega} J_c(P(x, t), k(x, t)) \, dx$ (cf. [BX08], who argue that they use periodic BC to exclude effects induced by the conditions at the end points. However, from a modeling point of view Neumann BC are more natural. Moreover, this point does not touch our argument that it is necessary to analyze the global behavior of the optimally controlled system.

Using Pontryagin’s Maximum Principle for PDEs, see e.g., [BX08, Trö09], with the current value local Hamiltonian

$$H(P, k, \lambda) = J_c(P, k) + q \left( k - bP + \frac{P^2}{1 + P^2} + D\Delta P \right)$$

the canonical system for (13) becomes

$$\partial_t P(x, t) = k(x, t) - bP(x, t) + \frac{P(x, t)^2}{1 + P(x, t)^2} + D\Delta P(x, t),$$

$$\partial_n P(x, t)|_{\partial \Omega} = 0, \quad P(x, t)|_{t=0} = P_0(x), \quad x \in \Omega \subset \mathbb{R}^d,$$

where $\Delta = \partial^2_{x_1} + \ldots + \partial^2_{x_d}$. We mostly focus on $\Omega = (-L, L)$ a real interval, but also give an outlook to 2D, see §2.5. We formulate the problem with Neumann (zero flux) boundary conditions (BC) in (13d) instead of the periodic BC in 1D in [BX08], who argue that they use periodic BC to exclude effects induced by the conditions at the end points. However, from a modeling point of view Neumann BC are more natural. Moreover, this point does not touch our argument that it is necessary to analyze the global behavior of the optimally controlled system.
with \( k(x,t) = -\frac{1}{q(x,t)} \), and the limiting intertemporal transversality condition
\[
\lim_{t \to \infty} e^{-rt} \int_\Omega q(x,t)P(x,t)dx = 0. \tag{16}
\]

Analogous to Def. 1.1 we define

**Definition 1.4.** Let \((P^*(\cdot,\cdot), k^*(\cdot,\cdot), P_0(\cdot))\) be an optimal solution of problem (13), i.e. for every admissible \( k(\cdot,\cdot) \) and associated \( P(\cdot,\cdot) \) we have
\[
J(P_0(\cdot), k(\cdot,\cdot)) \leq J(P_0(\cdot), k^*(\cdot,\cdot), P_0) = V(P_0(\cdot)).
\]

Then \( k^*(\cdot,\cdot), P_0 \) is called a (distributed) optimal control, \( P^*(\cdot,\cdot) \) is called the associated distributed optimal (state) path, and
\[
\partial_t P(x,t) = k^*(x,t, P_0(x)) - bP(x,t) + \frac{P(x,t)^2}{1 + P(x,t)^2} + D\Delta P(x,t) \tag{17}
\]
\[
\partial_u P(x,t)|_{\partial \Omega} = 0 \tag{18}
\]
is called the optimal PDE. Again with a slight abuse of notation, \((P^*, k^*)\) is also called an optimal solution of (15), and an optimal stationary solution \((\hat{P}(\cdot), \hat{k}(\cdot))\) of (15) is called an OSS (optimal steady state). If \( \hat{P}(\cdot) \equiv \hat{P} \) then the optimal steady state is called a FOSS (flat optimal steady state), otherwise it is called a POSS (patterned optimal steady state).

For a stationary solution \((\hat{P}(\cdot), \hat{q}(\cdot))\) (or \((\hat{P}(\cdot), \hat{k}(\cdot))\)) of the canonical system (15) we additionally introduce the acronyms FCSS for a flat canonical steady state, i.e \( \hat{P}(\cdot) \equiv \hat{P} \), and PCSS (patterned canonical steady state) otherwise. As already noted in the Introduction, the first interesting observation is that (15) can have many stationary states, in particular patterned states arising from Turing like bifurcations. Thus, we first calculate bifurcation diagrams for (15), in 1D and 2D, finding 2 branches of FCSS solutions, and many branches of PCSS solutions.

We expect a solution of (13) to behave analogous to Prop. 1 (without a proof at the moment). Thus, we only consider solutions \( u(\cdot,\cdot) := (P(\cdot,\cdot), q(\cdot,\cdot)) \) of (15) that satisfy
\[
\lim_{t \to \infty} u(\cdot,t) = \hat{u}(\cdot) := \hat{u},
\]
where \( \hat{u}(\cdot) \) is a stationary solution of (15). For \( \hat{u} \) we then also need a version of the SPP. However, \( E_u(\hat{u}) \) (and \( W_u(\hat{u}) \)) are infinite dimensional. We circumvent this problem by requiring (10) and (11) after a spatial discretization, which turns (15) into a (very large) systems of ODEs again. See App. A for further discussion. It turns out that the only CSS for (15) with the (discretized) SPP are a subset of the FCSS and a few of the PCSS. We then determine a number of optimal paths for our two scenarios above by calculating a number of canonical paths ending at such steady states and comparing their objective values, if multiple candidates exist.

\(^3\)A strict mathematical proof of Pontryagin’s Maximum Principle for diffusion process over an infinite time horizon is still missing, specifically for the transversality condition (16). In [Tro09] a finite time horizon is considered and the proof for 1D spatial problems in [BX08] is only given on a heuristic base. See also [BCF13] for a recent discussion of Pontryagin’s Maximum Principle in OC problems for parabolic PDE and infinite time horizons. Thus, at the moment we apply Pontryagin’s Maximum Principle in a naive sense. We specifically assume, based on the results for the original shallow lake model, that the solution converges to a stationary solution of the canonical system and therefore make no use of the “critical” transversality condition (16). Even then it is in general not clear a priori that a maximum in (13a) exists, since the canonical system may have infinitely many steady states, but we stick to the traditional notation max instead of sup.
2 Numerical methods, and results

The general idea is to use a method of lines discretization of (15), i.e., approximate

\[ u(x, t) := (P(x, t), q(x, t)) = \sum_{i=1}^{2N} u_i(t) \phi_i(x), \quad (19) \]

where \((\phi_i)_{i=1,\ldots,2N}\) spans a subspace \(X_N\) of the phase space \(X\) of (15), e.g., here \(X = [H^1(\Omega)]^2\), and \((u_i, u_{N+i}), i = 1, \ldots, N\), are the expansion coefficients of \(P, q\), respectively. For \(u \in X\) and \(\Pi_N\) the projection of \(X\) onto \(X_N\), i.e. \(\Pi_N u = \sum_{i=1}^{2N} u_i(t) \phi_i(x)\), we require \(||\Pi_N u - u||_X \to 0\) as \(N \to \infty\). This converts (15) into a (high dimensional) ODE

\[ \dot{u}_i(t) = \tilde{G}(u), \quad u_i(0) = u_{0,i}, i = 1, \ldots, N, \quad (20a) \]

for the coefficient vector \(u = (u_i)_{i=1,\ldots,2N}\), where we have initial data for exactly half of the expansion coefficients. We augment (20a) with the approximate transversality condition

\[ u(T) \in E_s(\bar{u}), \quad (20b) \]

where \(\bar{u}\) is a steady state of (20a), and \(E_s(\bar{u})\) is spanned by the eigenvectors of \(\partial_u G\) belonging to eigenvalues with negative real parts. As in 0D we then need the SPP, i.e.

\[ \dim E_s(\bar{u}) = \dim E_u(\bar{u}) \quad (21) \]

to chose an arbitrary initial point in the state space. For a short discussion and possible extension of the SPP to PDEs see App. A.

One of the simplest discretization options for (19) would be a finite difference scheme, which has the advantage that we can directly use OCMat for (20a). However, here we opt for a FEM ansatz for (19), using the setting of pde2path [UWR14, DRUW14] based on the Matlab pdetoolbox, for two reasons:

1. We want to consider (13) and hence (15) also on general 2D domains, and, moreover, more general models where the state variables may be vector valued functions already, see §3, again in 1D or 2D. In all these cases, FD and the coding of the respective spatially discrete systems may become rather inconvenient, while pde2path provides convenient interfaces precisely for such systems. Moreover, for more complicated systems adaptive meshes may become important, which are more easily handled in a FEM discretization, and are already an integral part of pde2path.

2. As explained above, the canonical system may have many stationary states; it is thus desirable to use a continuation and bifurcation package to conveniently find CSS. The goal then is to “seamlessly” link the setting of pde2path for stationary problems with BVP solvers for (20a).

On the other hand, a drawback of spatial FEM discretizations is that the associated evolutionary problems have the natural form

\[ M \dot{u}(t) = -Ku(t) + MF(u(t)) =: G(u(t)), \quad (22) \]

where \(u = (u_i(t))_{i=1,\ldots,2N}\) are the nodal values, \(M \in \mathbb{R}^{2N \times 2N}\) and \(K \in \mathbb{R}^{2N \times 2N}\) are called the mass matrix and the stiffness matrix, respectively, and \(F : \mathbb{R}^{2N} \to \mathbb{R}^{2N}\) is the nonlinearity. Thus, \(M\) and \(K\) are large but sparse; the “-” sign in (22) comes from the convention that the Matlab pdetoolbox and hence pde2path discretize \(-\Delta\) as \(K\). The occurrence of \(M\) on the LHS of (22) means that it is not of the form (20a), and creates problems for the usage of standard BVP solvers. Of course, \(M\) is non–singular, and hence (22) can be rewritten as

\[ \dot{u} = -M^{-1}Ku + F(u), \quad (23) \]

while pde2path is designed for spatial 2D problems, it can also be run in a quasi 1D setting, see §2.2...
where for speed we can pre-calculate $M^{-1}K$. However, $M^{-1}$ is no longer sparse, and already for intermediate $N$ ($N > 1000$, say) this results in slow computations and in particular memory problems when using standard BVP solvers, which sort the Jacobian $-M^{-1}K + \partial_u F$ from each time-slice $t_0, \ldots, t_m$ into a big Jacobian for the BVP problem. This can be alleviated by providing an approximate Jacobian $\hat{J} = -A + \partial_u F$, where $A$ approximates $M^{-1}K$ via lumping, i.e. we drop entries from $M^{-1}K$ below a certain size $\delta$. Of course, there is a tradeoff between accuracy of $\hat{J}$ and the number of its nonzeros.

We mainly experimented with the Matlab solvers bvp4c and similar, for instance the adaptations of bvp4c already implemented in OCMat, and the solver TOM [MS02, MT04, MST09]. It turned out, that TOM worked best in the “lumped” setting. Moreover, we could modify TOM in an easy ad hoc way to handle $M$ on the left hand side, and a new official release of TOM is scheduled that also uses $M$ [Maz15]. For now we use our modified TOM as follows: the right hand side of (22) is implemented as a function $f=rhs(t,u)$, which is simply a wrapper to call the respective implementation of the right hand side in pde2path, and where $t$ is a dummy argument since (22) is autonomous. For speedup it is advisable (in fact, mandatory for larger scale problems) to avoid numerical differentiation and hence to pass a Jacobian function $J=fjac(t,u)$ to TOM. This is generically very easy as pde2path in most cases provides a fast and easy way to assemble $J$. See also Remark 2.2 concerning the overall performance of our approach.

### 2.1 The algorithm for the computation of a path to a CSS satisfying the SPP

Let $\hat{u}$ satisfy the SPP. Then, to calculate CS-paths from a given state $P_0$ that converge to $\hat{u}$ we solve the time-normalized (see Remark 2.1) two-point BVP

\begin{align}
M \dot{u}(t) &= TG(u(t)), \quad t \in [0,1] \\
P_i(0) &= P_{0,i}, \quad i = 1,\ldots,N, \quad (N \text{ left BC}), \\
\Psi^T(u(1) - \hat{u}) &= 0 \in \mathbb{R}^N \quad (N \text{ right BC}),
\end{align}

with $\Psi^T(u - \hat{u}) = 0$ for $u \in E_s(\hat{u})$, and where $T$ is the chosen truncation time. The calculation of $\Psi$ at startup, which for large $N$ turns out to be one of the bottlenecks of the algorithm, also gives a lower bound for the time scale $T$ via $T \geq \frac{1}{\Re \mu_1}$, where $\mu_1$ is the eigenvalue with largest negative real part, i.e., gives the slowest direction of the stable eigenspace of $\hat{u}$. In the simulations below, we typically use $T$ between 50 and 100. In general, a numerical algorithm will not successfully solve problem (24) for an arbitrary initial distribution $P_{0,i}, i = 1,\ldots,N$. Therefore we embed problem (24) into a family of problems replacing (24b) by

\begin{align}
P_i(0) &= \alpha P_{0,i} + (1 - \alpha) P_{1,i}, \quad i = 1,\ldots,N, \quad \alpha \in [0,1],
\end{align}

where we assume that the solution with $P_i(0) = P_{1,i}$ is known, at least approximately; this holds, e.g., for $P_1$ close to $\hat{P}$. This problem is solved by the algorithm summarized in Table 1.

There are more sophisticated variants of the simple continuation in Step 2 of Table 1 (some of which are implemented in OCMat), but the simple version in general works well for the problems we considered. Nevertheless, it may be that no solution of (24a), (24c) and (24d) is found for $\alpha > \alpha_0$ for some $\alpha_0 < 1$, i.e., that the continuation to the intended initial point fails. In that case usually the BVP problem undergoes a fold bifurcation. We then use an adapted continuation step 3’ that allows us to continue solutions around the fold.

**Remark 2.1.** When repeatedly solving the BVP (24) within a continuation process it is assumed that the time scale $T$ is large enough to guarantee that $\|u(1) - \hat{u}\|_2$ remains satisfactorily small. In some cases this assumption is violated. For an example see Sec. 2.3 where, during a continuation

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5see also http://www.dm.uniba.it/~mazzia/bvp/index.html
Step 0 (selection of \( \hat{u} \) and implementation of (24c)). Given \( \hat{u} \) we solve the generalized adjoint EVP \( \partial_u G(\hat{u})^T \Phi = \Lambda M \Phi \) for the eigenvalues \( \Lambda \) and (adjoint) eigenvectors \( \Phi \), which also gives the defect \( d(\hat{u}) \). If \( d(\hat{u}) = 0 \), then from \( \Phi \in \mathbb{C}^{2N \times 2N} \) we generate a real base of \( E_\alpha(\hat{u}) \) which we sort into the matrix \( \Psi \in \mathbb{R}^{2N \times N} \).

Step 1 (selection of initial mesh). To start the BVP solver we need an initial guess \( u(t) \) on a suitable initial grid \( 0 = t_0 < t_1 < \ldots < t_m = 1 \). As we expect the main variation near \( t = 0 \) we typically use a finer grid near \( t = 0 \). This is a question of startup, as TOM afterwards uses its own mesh-adaption strategy, but a good initial–mesh (and initial–guess) helps a lot. Typically, we choose \( m = 20 \) at startup.

Step 2 (initial guess). A good initial guess \( P_1(0) = P_{1,i} \) is often difficult to find. If we do not already know a solution from a previous step we start with a solution we already have at hand. Namely the steady state \( u(\cdot) \equiv \hat{u} \), setting \( P_1 = \hat{P} \) and \( u(t_j) = \hat{u}, \ j = 1, \ldots, m \).

Step 3 (solution and continuation). We try to increase \( \alpha \) in small steps \( \delta \) to \( \alpha = 1 \), in each step using the previous solution as the new initial guess, often trying \( \delta = 1/4 \). After thus having computed the first two solutions we may use a secant predictor for the subsequent steps.

Step 3’ (solution and continuation). If the continuation fails for \( \alpha > \alpha_0 \) with \( \alpha_0 < 1 \) we use a modified BVP, letting \( \alpha \) be a free parameter and using \( \delta \) as pseudo–arclength. Since TOM does not allow free parameters we add the dummy ODE \( \dot{\alpha} = 0 \), and BCs at continuation step \( n \),

\[
\langle s, (u(0) - u^{(n-1)}(0)) \rangle + s_\alpha (\alpha - \alpha^{(n-1)}) = \delta,
\]

with \( u^{(n-1)}(\cdot) \) the solution from the previous continuation step \( n-1 \), and \( (s, s_\alpha) \in \mathbb{R}^{2N} \times \mathbb{R} \) appropriately chosen with \( \| (s, s_\alpha) \|_* = 1 \), where \( \| \cdot \|_* \) is a suitable norm in \( \mathbb{R}^{2N+1} \), which may contain different weighting between \( s \) and \( s_\alpha \). For \( s = 0 \) and \( s_\alpha = 1 \) we find the procedure of continuation step 3. Using

\[
s = \xi (u^{(n-1)}(0) - u^{(n-2)}(0))/\|u^{(n-1)}(0) - u^{(n-2)}(0)\|_2 \quad \text{and} \quad s_\alpha = 1 - \xi
\]

with small \( \xi \) and a secant predictor similarly based on \( (s, s_\alpha) \) allows to continue the solution around folds, see [GCF+08, §7.2.2]. In order to give equal weight to the parameter \( \alpha \) and the state/costate vector \( u \) here we typically choose \( \xi = 1/N \).

Table 1: The continuation–algorithm iscont (Initial State Continuation); Steps 0-2 are preparatory, Step 3 or 3’ is repeated.

process, the initial point \( u(0) \) approaches a defective CSS. Therefore, the time interval for which the path stays in the neighborhood of this CSS increases. The normalization of the time interval \([0,T]\) to \([0,1]\) allows us to consider \( T \) as a free variable, and for a fixed distance \( \varepsilon > 0 \) we add the auxiliary boundary condition

\[
\|u(1) - \hat{u}\|_2 = \varepsilon
\]

to the BVP (24). This guarantees that the distance to the equilibrium remains small and the time is accordingly adapted.

Remark 2.2. iscont works fast in 1D, and for small to intermediate meshes in 2D. More specifically, in 1D we use between \( 2N = 100 \) and \( 200 \) spatial degrees of freedom (DoF), and up to \( m = 100 \) points for the time discretization, and a full continuation with iscont is generically a matter of seconds on a desktop PC. In 2D we used meshes with up to \( 2N = 4000 \) spatial DoF and \( m = 50 \), hence \( 2 \times 10^5 \) total DoF, and then a single continuation step on iscont can take up to a minute. However, another bottleneck for large \( N \) becomes the calculation of \( \Psi \) at startup, which for \( 2N = 4000 \) is on the order
of a few minutes. Finally we remark that moderate to large scales are not a problem for \texttt{pde2path}: for instance, in [UW14] we treat problems with up to $5 \times 10^5$ DoF, with runtimes of about 30 minutes on a desktop PC for extended branches of several hundreds of stationary solutions.

\textbf{Remark 2.3.} A 0D CSS immediately yields a CSS in higher space dimensions. For comparison between different space dimensions, in the bifurcation diagrams we use the normalized $L^2$ norm, i.e., henceforth, $\|P\|_2 := \|P\|_{L^2(\Omega)}$, and in the table in Fig. 1 we present averaged values, i.e.,

$$\langle P \rangle := \frac{1}{|\Omega|} \int_{\Omega} P(x) \, dx, \quad \langle k \rangle := \frac{1}{|\Omega|} \int_{\Omega} k(x) \, dx.$$  \hfill (26)

Similiarly, we consider the spatially normalized objective values

$$J_{ca}(P, k) := \langle J_{c}(P(\cdot), k(\cdot)) \rangle \quad \text{and} \quad \bar{J}(P_0(\cdot), k(\cdot, \cdot)) := \frac{1}{|\Omega|} J(P_0(\cdot), k(\cdot, \cdot)), \hfill (27)$$

and to take the finite truncation time $T$ into account we let

$$\tilde{J}(k(\cdot), T) := \bar{J}(P_0(\cdot), k(\cdot, \cdot)) + e^{-rT} J_{ca}(P(T), k(T)). \hfill (28)$$

Obviously, for $T \gg \frac{1}{r}$ the last term can be made arbitrarily small, while for CSS it yields the exact (discounted) objective value. In the following we drop the tilde in (28), and write, e.g., $J_{\tilde{u}}$ for the objective value of a CSS $\tilde{u}$, and, e.g., $J_{P_1 \rightarrow \ti{u}}$ for the CS–path which goes from $P_1$ to $\tilde{u}$.

\subsection*{2.2 Scenario 1 in 1D}

Recall that first we use \texttt{pde2path} to study the steady state system for (20a), i.e.,

$$0 = -\frac{1}{q(x)} - bP(x) + \frac{P(x)^2}{1 + P(x)^2} + D\Delta P(x), \quad \hfill (29a)$$

$$0 = 2cP(x) + q(x) \left( r + b - \frac{2P(x)}{(1 + P(x))^2} \right) - D\Delta q(x), \quad \hfill (29b)$$

$$\partial_n P(x)|_{\partial\Omega} = 0, \quad \partial_n q(x)|_{\partial\Omega} = 0. \quad \hfill (29c)$$

In 1D we choose $\Omega = (-L, L) \times (\delta_y, \delta_y)$ with Neumann BC on all boundaries and small $\delta_y$ such that we can use just two grid–points in $y = x_2$–direction and the solutions will be constant in $y$; this we call a quasi 1D setup. It is clear that the steady states of the canonical system for the 0D model (1) are FCSS of (29). For easy reference we introduce the acronyms in Table 2.

\begin{table}[h]
\centering
\begin{tabular}{ll}
name & description \\
FSM & Flat State Muddy, the upper FCSS branch with a high phosphor load $P$ \\
FSI & Flat State Intermediate, the upper half of the second FCSS branch, intermediate $P$ \\
FSC & Flat State Clean, the lower half of the second FCSS branch, low $P$ \\
\end{tabular}
\caption{Classification of the FCSS branches, see also Fig.1.}
\end{table}

Following [BX08] and using \texttt{pde2path} we search for PCSS bifurcating from FCSS. For this, the domain size $2L$ should be close to a multiple of $2\pi/k_c$, where $k_c$ is the wave number of a Turing bifurcation. The parameters in (2), with $b$ near 0.7, yield $k_c \approx 0.44$ [BX08], and for simplicity we then choose $L = 2\pi/0.44 \approx 14.28$. 

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We continue the FSI branch in \( b \), find a number of Turing bifurcations, and follow four of these; see Fig. 1a, b for the bifurcation diagram(s), and (c) for example solutions\(^6\). On the branches \( p_1, p_2, \) and \( p_3 \) there are secondary bifurcations, not further considered here. For the subsequent examples we focus on \( b = 0.75 \) and \( b = 0.65 \), check the SPP (Def. 1.3) for all steady states and find it only to be fulfilled for the FSM, for the FSC, and for some points on the \( p_1 \) branch, e.g., at point 71 between the folds (see Fig. 1).

(a) BD of CSS, (normalized) \( L^2 \) norm over \( b \)  
(b) BD, current values \( J_{c,a} \)  
(c) example CSS

(d) Characteristics of points in (a)-(c).

| name | \langle P \rangle | \langle k \rangle | \( J_a \) | \( d \) | name | \langle P \rangle | \langle k \rangle | \( J_a \) | \( d \) |
|------|-----------------|-----------------|--------|------|------|-----------------|-----------------|--------|------|
| FSM/pt20 | 1.22 | 0.32 | -63.11 | 0 | p1/pt16 | 0.61 | 0.14 | -74.83 | -1 |
| FSM/pt11 | 1.44 | 0.26 | -79.28 | 0 | p1/pt71 | 1.24 | 0.22 | -78.93 | 0 |
| FSI/pt36 | 0.87 | 0.13 | -79.47 | -5 | p2/pt16 | 0.76 | 0.15 | -76.70 | -2 |
| FSC/pt12 | 0.45 | 0.12 | -72.95 | 0 | p3/pt19 | 1.02 | 0.17 | -79.48 | -3 |

Figure 1: Basic bifurcation diagrams, example plots and characteristic values of selected CSS.

For \( b = 0.75 \) only the FSM steady state \( \text{FSM/} \text{pt20} \) exists. It has the SPP, we can reach it from an arbitrary initial state \( P_0 \), and thus it is a globally stable FOSS.

For \( b = 0.65 \) seven CSS are marked in Fig. 1a, and characterized in the table, where only three satisfy the SPP. These are the FSC (which has the maximal value among these CSS), the FSM, and the PCSS \( p_1/pt71 \), subsequently denoted as \( \hat{u}_{PS} (\cdot) \). Next we numerically analyze which of these CSS belong to optimal paths.

**PCSS not satisfying the SPP.** From the analysis of non-distributed optimal control problems we know that steady states that do not satisfy the SPP can nevertheless be optimal. First we compare the objective value of a CSS, e.g., the PCSS \( \hat{u}_{PS} (\cdot) \) \( p_3/pt16 \), not satisfying the SPP, with that of all \( t \)-dependent canonical paths \( u_i (\cdot,0) = P_{PS} (\cdot), \ i \in \{\text{FSC, FSM, PS}\} \) and

\[
\lim_{t \to \infty} u_i (\cdot, t) = \hat{u}_i (\cdot), \quad i \in \{\text{FSC, FSM, PS}\}.
\]

For the objective values we write \( J_{PS}^\cdot \) for the CSS, and, e.g., \( J_{PS}^{FSM} \), for the canonical path which goes from \( P_{PS} \) to \( u_{FSM} \). The optimal solution for \( P_0 = P_{PS} \) has to satisfy

\[
V (P_{PS}) = \max \{ J_{PS} \ , \ J_{PS}^{FSM} \ , \ J_{PS}^{FSM} \ \to \ \text{FSC} \ , \ J_{PS}^{FSM} \ \to \ \text{PS} \}.
\]

\(^6\)The notation, e.g., \( p1/pt16 \) follows the pde2path scheme, e.g.: continuation step 16 on the branch p1 is stored in folder p1 and file pt16.mat.
To calculate the canonical paths for \( i \neq \text{PS}^- \) we use \texttt{iscont} with the initial state \( P_0 = \hat{P}_{\text{PS}^-} \) as the continuation target.

Exemplarily we carry out this analysis for the two humped PCSS solution \( p3/pt19 \) as the starting PCSS. See Fig. 2a–c for plots of the canonical paths, and (d) for plots of some norms along the paths, which show that and how fast \( u(t) \) (including the co–states \( q \)) converges to \( \hat{u} \). In all cases we find without problems canonical paths to both FCSS and the PCSS; in particular the path to FSM is rather quick. Interestingly, the control \( k \) taking the \( P \) from the starting CSS to the target CSS is initially rather close to the control of the starting CSS; see §2.4 for short remarks on economic interpretations.

For the objective values we find, up to 2 significant digits,

\[
J_{PS^-} = -79.48 < J_{PS^- \to \text{FSC}} = -78.24 < J_{PS^- \to \text{PS}} = -78.19 < J_{PS^- \to \text{FSM}} = -77.5. \tag{31}
\]

Thus, the optimal solution is the path converging to \( \hat{u}_{\text{FSM}} \). Repeating these steps for every PCSS not satisfying the SPP we find that these are always dominated by paths converging to one of the FCSS. Therefore, only \( \hat{u}_{\text{FSC}}, \hat{u}_{\text{FSM}} \) and \( \hat{u}_{\text{PS}} \) remain as candidates for OSS.

(a) CS path from \( p3/pt19 \) to FSC
(b) CS path from \( p3/pt19 \) to FSM
(c) CS path from \( p3/pt19 \) to PS
(d) diagnostics for a) and c)

Figure 2: Canonical paths from the (state values of) PCSS\(^-\) \( p3/pt19 \) to FSC (a), FSM (b), and PS (c) at \( b = 0.65 \), and typical path diagnostics (d).

**Determining optimal steady states.** We proceed in three steps. First we search for a \( t \)–dependent canonical path starting at \( \hat{P}_{\text{PS}^-}(\cdot) \) and converging to \( \hat{u}_{\text{FSC}} \). In the second step we repeat that for \( \hat{u}_{\text{FSM}} \), and in the last step we check if both or only one of the FCSS are optimal.\(^7\)

**Paths between \( \hat{P}_{\text{PS}^-}(\cdot) \) and \( \hat{P}_{\text{FSC}}(\cdot) \) – a Skiba candidate.** Using \texttt{iscont} to get a canonical path starting at \( \hat{P}_{\text{PS}} \) and converging to the FSC it turns out that the continuation (24d), i.e.,

\[
P_\alpha(0) := \alpha P_{\text{PS}} + (1 - \alpha) P_{\text{FSC}}, \tag{32}
\]

\(^7\)The second step reveals that the first step is superfluous, but for a different set of parameter values it may become relevant.
yields a fold around $\alpha \approx 0.6$, see the blue curve in Fig. 3a), and that no canonical path that starts at $P_{PS}$ and converges to $u_{FSC}$ exists. Instead multiple solutions, that converge to $u_{FSC}$, exist for initial distributions of the form (24d) with $\alpha \in [0.6, 0.71]$; two examples are shown in Fig. 3b, and their diagnostics in (c).

Similarly, trying to continue to a solution that starts at $\hat{P}_{FSC}(\cdot)$ and connects to $u_{FSM}$ yields a fold (green curve in (a)), and no such solution exists. However, the solutions returned during the continuation process allow us to determine and compare the respective objective values yielding that there exists a specific initial distribution where the objective values are equal, given by the intersection of the green and blue curves in Fig. 3a. This initial distribution $P_S$ is called a Skiba or indifference threshold point, well known from the non-distributed optimal control problems. The corresponding solutions $u$ starting at the Skiba distribution (red curve) are depicted in Fig. 3d. By the definition of a Skiba distribution $P(0)$ is the same for both solutions, whereas the controls $k(0)$ are different. Thus, from an economic point of view both solutions are equally optimal. In any case, to assure that these solutions are optimal we have to prove that no other dominating solution exists. Thus in a last step we calculate the objective values of $u_{FSM}$ and the paths converging to it.

\[ \text{Figure 3: Canonical paths to various CSS for } b = 0.65, \text{ and illustration of some Skiba points; see text for details.} \]

- (a) $J_{i,a}$ for FSC target
- (b) Two paths to FSC for $\alpha = 0.6$
- (c) Diagn. for left and right paths in (b)
- (d) A Skiba candidate between $P_{PS}$ and FSC
- (e) $J_{i,a}$ for FSM target
- (f) Dominating path to FSM
- (g) 0D Shallow Lake
- (h) Homog. Skiba point and paths to FSC and FSM
- (i) A patterned Skiba point between FSC and FSM
From $\hat{P}_{\text{PS}}(\cdot)$ to $\hat{u}_{\text{FSM}}$. In that case the continuation is successful and we find a path starting at $\hat{P}_{\text{PS}}(\cdot)$ and converging to $(\hat{P}_{\text{FSM}}(\cdot), \hat{q}_{\text{FSM}}(\cdot))$. Comparing the objective values reveals that the PCSS is dominated by the solution converging to the FSM, see Fig. 3e and 3f. Thus, the PCSS is ruled out as an optimal steady state, and therefore we a posteriori identify $P_S$ as only a Skiba candidate as it does not separate two optimal steady states.

A Skiba manifold between $\hat{P}_{\text{FSM}}(\cdot)$ and $\hat{P}_{\text{FSC}}(\cdot)$. It is well known that in 0D the FSC and FSM are only locally stable with regions of attractions separated by a Skiba manifold (parametrized by, e.g., $b$) of homogeneous solutions, [KW10], see Fig. 3g for our case $b = 0.65$. Of course, this also yields a homogeneous Skiba distribution in 1D, see 3h. More generally we may expect the regions of attractions of the FSC and the FSM to be separated by an (in the continuum limit infinite dimensional) Skiba manifold $M_S$, for fixed $b$.

A continuation process, analogous to the non-distributed case, see [Gra12], could be used to approximate this manifold $M_S$. However, to find a nonhomogeneous example point on that manifold, here we can readily combine Fig. 3a and 3e, to find a Skiba point of the form

$$P_{\text{Skiba}} = \alpha\hat{P}_{\text{FSC}} + (1 - \alpha)\hat{P}_{\text{PS}}$$

see Fig. 3i for paths to the FSC and the FSM yielding the same $J = -76.3$.

Summary for Scenario 1. The picture that emerges in Scenario 1 is as follows: for $b > b_{\text{fold}} \approx 0.727$ the FSM as the only CSS is the globally stable FOSS, while for $b < b_{\text{fold}}$ there exist multiple CSS. Specifically for $b = 0.65$, $\hat{u}_{\text{FSC}}, \hat{u}_{\text{FSM}}$ and one of the PCSS have the SPP, but only $\hat{u}_{\text{FSC}}$ and $\hat{u}_{\text{FSM}}$ are optimal, and in particular no POSS exists. The FOSS FSC and FSM are separated by a (presumably rather complicated) Skiba manifold $M_S$, and Fig. 3h and 3i show just 2 examples of points on $M_S$.

2.3 Scenario 2 in 1D

A parameter regime where we can find POSS solutions for (15) is given by Scenario 2 with a larger discount rate, and larger ecological costs, i.e., $r = 0.3, b = 0.55, D = 0.5$, and $\gamma$ near 3 as the primary bifurcation parameter. Bifurcation diagrams in this regime are shown in Fig. 4, together with some example PCSS and values at $\gamma = 3.25$. Again we have three FCSS, namely the clean (FSC), intermediate (FSI), and muddy (FSM) ones, with FSC and FSM satisfying the SPP, and three PCSS, none of them satisfying the SPP.9

Again the FSI, that does not satisfy the SPP, in 0D separates the regions of attraction of the locally stable FSC and FSM. In a next step we numerically test if the PCSS can also act as separators and are thus potentially POSS. As an example we take the PCSS $q2/pt13$ and denoted henceforth as $u_{\text{PS}}$, and try to find canonical paths, that start at $\hat{P}_{\text{PS}}(\cdot)$ and converge to either the FSC or the FSM. During the continuation process for a fixed truncation time $T$ the distance between the last point of the canonical path and the target FCSS starts to increase. Geometrically this means that the solution ends at the stable eigenspace but time becomes to short to end “near” the equilibrium. Therefore we use the extended BVP discussed in Remark 2.1.

For the state variable, the results of these computation are shown in Fig. 5. Panel (a) shows the time paths of the spatial norms for the last computed solutions, converging to the FOSS (blue curves), starting closely to the patterned state $\hat{P}_{\text{PS}}(\cdot)$ (magenta). It now becomes obvious why a fixed time horizon $T$ fails to solve the problem. For an initial point near the PCSS, the canonical path stays near the PCSS for a long time, before it converges to one of the FOSS. Thus, it is not possible to find a solution starting at $\hat{P}_{\text{PS}}$ and converging to one of the FOSS. In fact the canonical paths with $P = \hat{P}_{\text{PS}}$ is the constant PCSS path. Thus it is a POSS, which however is not locally stable. Figures

\[^9\text{Of course the BD is qualitatively different in the sense that in } \gamma \text{ the FSC, FSI and FSM now are really on one } S\text{-shaped branch, and the PCSS branches reconnect to this FCSS branch.}\]
(a) BD of CSS  (b) BD, current values $J_{c,a}$  (c) example CSS

(d) Characteristics of points in (a)-(c).

| name          | $\langle P \rangle$ | $\langle k \rangle$ | $J_a$ | $d$ |
|---------------|---------------------|---------------------|-------|-----|
| FSM/pt14      | 1.08                | 0.06                | -22.25| 0   |
| FSC/pt57      | 0.45                | 0.08                | -10.59| 0   |
| FSI/pt34      | 0.81                | 0.05                | -17.16| -4  |
| q2/pt13       | 0.90                | 0.05                | -18.92| -2  |

Figure 4: Bifurcation diagrams for Scenario 2, and example plots and values.

(b) and (c) show $P$ for two canonical paths starting near $\hat{P}_S$ and converging to the FSC and the FSM, respectively, illustrating how this POSS acts as a separator.

To be precise, what we have numerically proved so far is that one of the equilibria not satisfying the SPP is optimal. To prove the optimality of the considered PCSS it would be necessary also to show that no path exists that starts at $\hat{P}_S$ and converges to one of the other equilibria. For this, the defect of the target equilibria plays a crucial role, because it determines (at least in the discretization) the dimension of the stable manifold. The defect of the intermediate FCSS is $-4$ and therefore stronger than the defect for any of the PCSS. Thus, generically no solution path starting at $\hat{P}_S$ and converging to this FCSS exists. Therefore, at least one of the PCSS is optimal.

For completeness we note that in [Gra15] the problem with $c = 3.0825$ is analyzed. In that case a PCSS satisfying the SPP exists and turns out to be a locally stable POSS; see [Gra15] for details.

Figure 5: Solution paths starting near the POSS (magenta).

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10 Using a finite difference approach that allows an immediate application of OCMat to analyze the discrete version of problem (13) in 1D.
2.4 Remarks on the economic interpretation

The economic interpretation of our numerical results is not the main topic of this article, and we therefore do not give a detailed discussion. However, to show that the results make sense intuitively we briefly discuss two examples, i.e., the cases $c = 2.5$ and $c = 3.6$ of Scenario 2. Relatively small environmental costs $c$ yield a globally stable muddy FOSS and high costs a globally stable clean FOSS.

Examples of optimal paths starting at the initial distribution $\hat{P}$, corresponding to the state values of the PCSS from the previous section are given in Fig. 6. For high $c$ the initial $P$ lies above the long run $P$. Therefore, the intensity $k$ of farming is chosen in a way that reduces and flattens $P$ concentration, see (a). In particular, near the equilibrium the farming intensity is relatively high where phosphorous is low and vice versa. Note that initially this behavior is inverted.

In the low $c$ regime the initial $P$ lies below the long run concentration, and the optimal strategy follows a different and not entirely intuitive rule: high $k$ at already high $P$, and vice versa, until $P$ reaches its higher level and is flattened out by diffusion, shown in (b).

To gain deeper insight into the complexity of optimal farming strategies it should be interesting to also study the influence of the diffusion coefficient $D$, including a more detailed discussion in the cases where patterned equilibria exist. However, this we postpone to future work, and here conclude with an outlook on 2D results.

\[ J(\text{PCSS}) = -77.53 < J(\text{PCSS} \rightarrow \text{FSC}) = -76.23 < J(\text{FSC}) = -72.97. \]  

Thus, this PCSS is not optimal, and neither is any other one we checked. Using the methods from §2.2 it is now of course also possible to find points with a genuine $x$ and $y$ dependence on the Skiba manifold separating FSC and FSM, but here we skip this presentation.

The behaviour and economic interpretation of the canonical path from the PCSS to the FSC in Fig. 8 is rather similar to the convergence to the FSC in §2.4: At least after a short transient the

\begin{center}
\textbf{Figure 6: Solution paths $P, k$ for high ($c = 3.6$) and low ($c = 2.5$) environmental costs.}
\end{center}

2.5 Outlook: 2D results

In §2.2 we first used pde2path to find CSS, in particular PCSS, for the quasi 1D problem (29), and afterwards used TOM for (23) with the continuation algorithm from Table 1 to calculate canonical paths involving these CSS. In Figures 7 and 8 we give some first results illustrating this approach in 2D. Here we consider (15) on the domain $\Omega = (-L,L) \times (-L/2,L/2)$, $L = 2\pi/0.44$ as before, with a rather coarse mesh of $40 \times 20$ points, hence approximately 1600 DoF. The FCSS branches are of course the same as in 1D (or 0D), and again at the end of the FSI branch we find a number of Turing like bifurcations. In Fig. 7(a),(b) we only present the “new” patterned branches, i.e., those with a genuine $x$ and $y$ dependence.

These new bifurcating PCSS again do not fulfill the SPP. As an example for a canonical path, in Fig. 8 we present snapshots from a path from $P$ of the PCSS $h2/pt17$ to the FSC (see also www.staff.uni-oldenburg.de/hannes.uecker/pde2path for the movie), which yields a higher $J$ than in the PCSS, i.e.,

\[ J(\text{PCSS}) = -77.53 < J(\text{PCSS} \rightarrow \text{FSC}) = -76.23 < J(\text{FSC}) = -72.97. \]  

Thus, this PCSS is not optimal, and neither is any other one we checked. Using the methods from §2.2 it is now of course also possible to find points with a genuine $x$ and $y$ dependence on the Skiba manifold separating FSC and FSM, but here we skip this presentation.

The behaviour and economic interpretation of the canonical path from the PCSS to the FSC in Fig. 8 is rather similar to the convergence to the FSC in §2.4: At least after a short transient the
optimal strategy is to give a high phosphor load $k$ where $P$ is below the limit value $\hat{P}_{\text{FSC}}$ (south-west and north-east corners of the domain), but initially there also is a high $k$ at high $P$ values (north-west and south-east corners). Again we postpone a more detailed study of this including the influence on $D$ to future work.

3 Discussion

There is strong evidence that locally stable optimal PCSS are rare for the shallow lake model (13). On the spatially discrete level, this conjecture is based on the observation that the discretized PCSS typically lack the SPP (21). Hence their stable manifolds do not cover the entire state space and the PCSS can therefore be excluded as a (locally stable) steady state of the optimal system. On the PDE level, this question cannot be answered at the moment since the pertinent manifolds are of infinite dimension, and further studies are necessary to clarify these concepts for PDEs.

Our results are intrinsically numerical, i.e., we first approximate the PDE by a large system of ODEs, where we can resort to our experience with non-distributed optimal control problems. However, we believe that our results can help to develop the theoretical concepts for distributed optimal control problems. This follows Oliver Heavisides’ dictum

“Mathematics is an experimental science, and definitions do not come first, but later on.”

On the applied side, some future steps are as follows: On the one hand we shall use our approach,
i.e., using pde2path to find CSS and afterwards TOM to find canonical paths, to give a more detailed discussion of the results from an economic point of view, including an analysis of the influence of the diffusion constant $D$. On the other hand, besides some other OC problems with a scalar state equation, we already started to apply the methods to more complicated OC problems, where the uncontrolled system is already a system of PDEs exhibiting pattern formation. For instance, in [Uec15] we study the vegetation system from [BX10] and find that POSS dominate in large parameter regimes. Other natural candidates, i.e., systems with natural objective functions and controls, are related vegetation systems as in [SZvHM01, ZKY+13], or “crimo-taxis” systems as in [SBB10]. As these uncontrolled systems have stable patterned states, we strongly suspect that with controls they all have locally stable POSS in rather wide parameter ranges.

A SPP for PDEs

In this appendix we discuss the SPP (11) in a somewhat more general situation tailored to canonical systems coming from spatial discretizations of PDEs. Let $\hat{u} = (p, q) \in \mathbb{R}^{2n}$ be a stationary state of a canonical (ODE) system of the form

$$\frac{d}{dt} \begin{pmatrix} p \\ q \end{pmatrix} = F(p, q) := \begin{pmatrix} f(p, q) \\ pq - H_p(p, q) \end{pmatrix},$$

(35)

where $f = H_q$, and let $J = D_u F(\hat{u})$ be the Jacobian at $\hat{u}$. In [GCF+08, Thm 7.10] it is explained that the eigenvalues of $J$ are symmetric around $r/2$, i.e., that there exist $n$ complex numbers $\xi_i$ such that

$$\sigma(J) = \left\{ \frac{r}{2} \pm \xi_i : i = 1, \ldots, n \right\},$$

(36)

In detail, since $\det(J - \xi) = \det(J_r - (\xi - \frac{r}{2}))$ where

$$J_r := J - \frac{r}{2} = \begin{pmatrix} H_{pq} - \frac{r}{2} & H_{qq} \\ -H_{pp} & -H_{pq} + \frac{r}{2} \end{pmatrix},$$

(37)

we have that $\frac{r}{2} + \xi_i \in \mathbb{C}$ is an eigenvalue of $J$ if and only if $\xi_i$ is an eigenvalue of $J_r$. But $J_r$ has the structure $\begin{pmatrix} A & B \\ C & -A \end{pmatrix}$ with symmetric matrices $B, C \in \mathbb{R}^{n \times n}$, and as a consequence the eigenvalues of $J_r$ are $\xi_i = \pm \sqrt{\xi_i}$, $i = 1, \ldots, n$.

Now consider the distributed canonical system

$$\partial_t \begin{pmatrix} p(x, t) \\ q(x, t) \end{pmatrix} = F(p(x, t), q(x, t)) + \begin{pmatrix} D \Delta p(x, t) \\ -D \Delta q(x, t) \end{pmatrix},$$

(38)

where $D \in \mathbb{R}^{n \times n}$ is a diffusion matrix, i.e., positive definite. Let

$$\frac{d}{dt} u(t) = G(u(t)), \quad u \in \mathbb{R}^{2nN},$$

(39)

be the associated spatially discretized system with $N$ spatial points, where

$$u = (p(x_1), \ldots, p(x_N), q(x_1), \ldots, q(x_N)) \in \mathbb{R}^{2nN},$$

and let $\hat{u} \in \mathbb{R}^{2nN}$ be a steady state of (39). Then $J = D_u G(\hat{u})$ has the structure $J = -K + J_{local}$,
where $J_{\text{local}}$ has the block structure

$$J_{\text{local}} = \begin{pmatrix} H^1_{pq} & 0 & \ldots & 0 & H^1_{qq} & 0 & \ldots & 0 \\ 0 & H^2_{pq} & \ldots & 0 & 0 & H^2_{qq} & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & H^{N}_{qq} & 0 & 0 & \ldots & H^{N}_{qq} \\ -H^1_{pp} & 0 & \ldots & 0 & r - H^1_{qp} & 0 & \ldots & 0 \\ 0 & -H^2_{pp} & \ldots & 0 & 0 & r - H^2_{qp} & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & -H^{N}_{pp} & 0 & 0 & \ldots & r - H^{N}_{qp} \end{pmatrix},$$

(40)

composed of local matrices $H^1_{pq} := H_{pq}(x_j) := H_{pq}(p(x_j), q(x_j)), H^1_{pp}, H^1_{pp} \in \mathbb{R}^{n \times n}$, and $K = \begin{pmatrix} L & 0 \\ 0 & -L \end{pmatrix}$ with $L \in \mathbb{R}^{n \times n}$ coming from the discretization of $D\Delta$. The notation $K$ of course reflects the FEM background of the present paper, but the same structure $(L 0 \ -L)$ occurs for any discretization, in any space dimension, and for any $D$ not necessarily diagonal, i.e., containing cross diffusion.

It follows that again $\hat{\xi} + \xi_i$ is an eigenvalue of $J$ if and only if $\xi$ is an eigenvalue of $J_r := J - \frac{r}{2}$, where $J_r$ has the structure

$$J_r = \begin{pmatrix} A & B \\ C & -A \end{pmatrix},$$

with symmetric $B, C \in \mathbb{R}^{n \times n}$.

Applying [GCF+08, Lemma B.2, Lemma B.3] we obtain

**Theorem A.1.** Let $\hat{u}$ be a steady state of the spatially discretized distributed system (39), and let $J$ be the associated Jacobian. Then there exist $\xi_i \in \mathbb{C}$, $i = 1, \ldots, nN$, such that

$$\sigma(J) = \left\{ \frac{r}{2} \pm \xi_i : i = 1, \ldots, nN \right\}.$$ 

(41)

As a consequence, $\dim E_s(\hat{u}) \leq Nn$, and the only candidates $\hat{u}$ for right BC in (24c) are those with the SPP (11). Therefore we concentrate our search on these steady states, but have in mind that a steady state $\hat{u}_0$ (and its stable path) with $\dim E_s(\hat{u}_0) < N$ may play a role in building the boundary between different regions of attraction for locally stable steady states, see [KW10, GCF+08].

As a corollary we find a property that, on the discretized level, is equivalent to the SPP.

**Corollary A.2.** Let $\hat{u} \in \mathbb{R}^{2nN}$ be an equilibrium of the spatially discretized distributed system (39) and $r > 0$. Then $\hat{u}$ satisfies the SPP iff every eigenvalue $\xi$ of the according Jacobian $J(\hat{u})$ satisfies

$$\|\Re \xi - \frac{r}{2}\| > \frac{r}{2}. $$

(42)

**Remark A.3.** Theorem A.1 is formulated on the discretized level, and one might ask how it ultimately relates to the PDE. As a first step one can ask: Let a steady state $\hat{u} \in \mathbb{R}^{2nN}$ of (39) be an approximation of a PDE steady state $(\hat{p}, \hat{q}) \in X$ for (38), with $X \subset \{(p, q) : \Omega \to \mathbb{R}^{2n}\}$ some function space. If $\tilde{\hat{u}} \in \mathbb{R}^{2nN}$ is an approximation of $(\hat{p}, \hat{q})$ on a finer mesh $\tilde{N} > N$, or just a different mesh, do we have

$$nN - \dim E_s(\hat{u}) = n\tilde{N} - \dim E_s(\tilde{\hat{u}})$$

(43)

We do not want to go into the details here, but if $E_s(\hat{u}) = \emptyset$, i.e., $\sigma(J) \cap \{\Re \xi = 0\} = \emptyset$, then (43) is true, for large enough $N, \tilde{N}$. Given some $\hat{u}$, this can be easily tested numerically, and it is also clear heuristically from an analytical point of view. Refining $\hat{u}$ to $\tilde{\hat{u}}$ we essentially add high frequency modes to the FEM (or finite difference) mesh. These introduce the same number of additional eigenvalues at
large positive and negative $\xi$ for the linearization $\tilde{J}$, because $J_F(p,q) : X \to X$ is relatively compact with respect to the Laplacian, i.e., w.r.t. $(p,q) \mapsto (D\Delta p, -D\Delta q)$. On the other hand, the small eigenvalues $\mu_i$, $|\mu_i| < R$ for some fixed $R$, are only slightly perturbed, i.e., $|\mu_i - \tilde{\mu}_i| \leq C\|\hat{u}_* - \tilde{\hat{u}}\|$, where $\hat{u}_*$ is suitably defined, for instance by interpolating $\hat{u}$ to the mesh of $\tilde{\hat{u}}$. But $\|\hat{u}_* - \tilde{\hat{u}}\| \to 0$ as $N, \tilde{N} \to \infty$, which yields (43).

To make this rigorous, we need to define appropriate function spaces and study the approximation properties of the spatial discretization. This is easy, as the stationary problem for (38) can be written as an elliptic system, and hence $(p,q)$ is arbitrary smooth, but we omit the details here.

In fact, (42) can also be formulated on the PDE level and might therefore replace the SPP (11) for spatially distributed models. However, we also postpone an in depth analysis of the applicability of (42) to future work.

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