

Computational singular perturbation method for nonstandard slow-fast systems

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Abstract

The computational singular perturbation (CSP) method is an algorithm which iteratively approximates slow manifolds and fast fibers in multiple-timescale dynamical systems. Since its inception due to Lam and Goussis [27], the convergence of the CSP method has been explored in depth; however, rigorous applications have been confined to the standard framework, where the separation between ‘slow’ and ‘fast’ variables is made explicit in the dynamical system. This paper adapts the CSP method to *nonstandard* slow-fast systems having a normally hyperbolic attracting critical manifold. We give new formulas for the CSP method in this more general context, and provide the first concrete demonstrations of the method on genuinely nonstandard examples.

1 Introduction

Most systems in nature consist of processes that evolve on disparate timescales and the observed dynamics in such systems reflect these multiple timescale features as well. Mathematical models of such multiple timescale systems are considered singular perturbation problems with slow-fast (or two timescale) problems as the most common. Models of homogeneously mixed biochemical reactions such as substrate-enzyme or ligand-receptor kinetics are prime examples.

An interesting and pervasive feature of these biochemical reaction systems is the observed transition from transient fast kinetics to long-term slow kinetics, wherein the system settles onto a so-called *quasi-steady state* (QSS). Geometrically, this QSS is perceived as a lower dimensional *slow manifold*. Identifying

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such an attracting lower dimensional slow manifold provides the means to reduce the dimension of biochemical reaction systems. Such QSS reduction techniques are frequently employed in the biochemical literature with *Michaelis-Menten-type* laws [15] as prime examples; see e.g. [20].

The mathematical foundation to justify such a QSS reduction is given by Tikhonov's [42] respectively Fenichel's [7] work on normally hyperbolic attracting slow manifolds in singular perturbation problems. Goeke, Noethen, Stiefenhofer, and Walcher [10, 36, 41] have provided comprehensive discussions on the general setup of Fenichel's geometric singular perturbation theory (GSPT), with an emphasis on explaining when a QSS reduction is justified or when it leads to erroneous results.

Schauer and Heinrich [40] explored a homotopy approach to find QSS approximations in biochemical reaction networks, by formulating a perturbation problem in terms of a small parameter $\varepsilon > 0$ amplifying the ratio of magnitudes of slow and fast reaction rates.¹ After using stoichiometry to derive the dynamical system from the network, the fast reactions are grouped into a vector W , and slow into a vector V :

$$z' = NW(z) + \varepsilon RV(z), \quad (1)$$

with state vector $z \in \mathbb{R}^n$, N and R are constant stoichiometric matrices with full column rank $m_N, m_R < n$, and $\varepsilon > 0$ is the homotopy parameter. With this splitting, a k -dimensional manifold of stationary states (QSS), $1 \leq k < n$, can be identified in the singular limit $\varepsilon \rightarrow 0$,

$$S = \{z \in \mathbb{R}^n : NW(z) = 0 \Rightarrow W(z) = 0\}. \quad (2)$$

We emphasize here that the slow-fast splitting (1) is *nonstandard* from the point of view of GSPT in the sense that slow-fast reactions are distinguished rather than slow-fast variables. Nevertheless, the theory of Fenichel [7] still applies: under the appropriate geometric condition (see Section 2 for details), an invariant slow manifold S_ε perturbs from S for sufficiently small $\varepsilon > 0$.

As a motivating example, consider the following four-dimensional slime mold cell communication model [9]:

$$\begin{pmatrix} p' \\ d' \\ r' \\ b' \end{pmatrix} = \begin{pmatrix} 2 & 2 \\ 0 & 1 \\ 1 & 0 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} -k_5 r p^2 + k_{-5} b \\ -k_4 d p^2 + k_{-4}(c - d - r - b) \end{pmatrix} + \varepsilon \begin{pmatrix} k_3 - k_{-3} p + k_2 S b \\ -k_1 d + k_{-1} r \\ k_1 d - k_{-1} r \\ 0 \end{pmatrix} \quad (3)$$

Here, p refers to the concentration of cAMP; d and r represent transmembrane receptors; and b refers to the bound state of r . The parameters $k_i \geq 0$ are constant reaction rates, the parameter $c \geq 0$ represents a conserved quantity that arises from the model reduction of the original five-dimensional model due

¹We note that a small perturbation parameter $\varepsilon > 0$ could be properly identified via dimensional analysis.

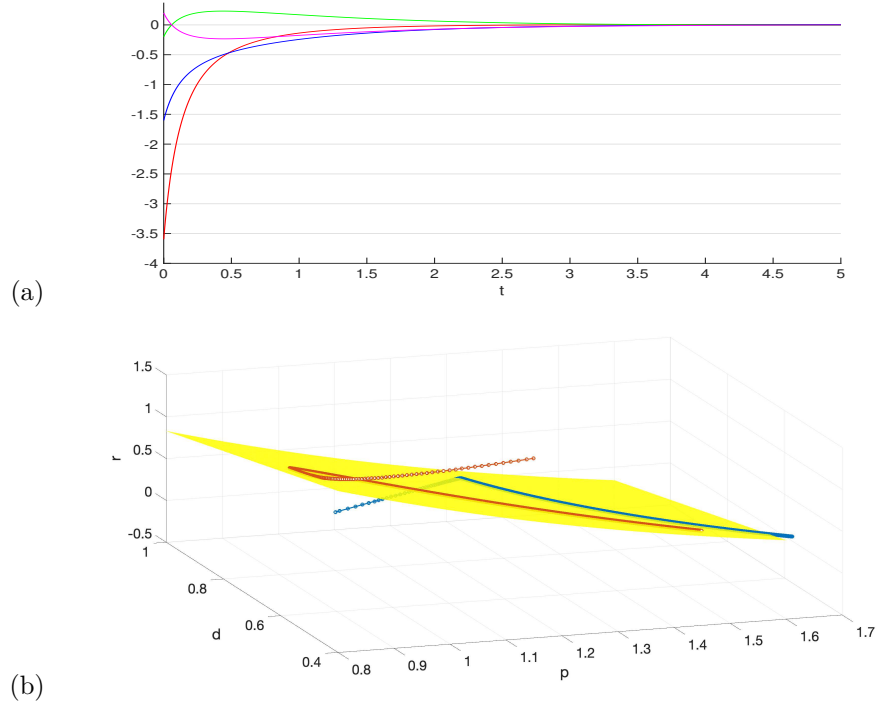


Figure 1: System (3) with $\varepsilon = 0.01$, $k_i = S = 1$, $c = 3$ and initial conditions: $(p, d, r, b) = (1, 0.8, 0.6, 0.4)$; (a) Time series of the velocities p' , d' , r' , b' (respectively in red, blue, green, magenta). (b) Projection onto (p, d, r) space of two trajectory segments together with a portion of the manifold of equilibria defined by (4). Initial conditions: blue, $(p, d, r, b) = (1, 0.8, 0.6, 0.4)$; red, $(p, d, r, b) = (1.2, 0.5, 1.4, 0.4)$.

to Stiefenhofer [41], and the parameter $S \geq 0$ denotes the concentration of ATP which is assumed to be constant. This system contains a two-dimensional manifold of equilibria given as a graph

$$S = \{(p, d, r, b) \in \mathbb{R}^4 : (r, b) = \psi(p, d)\} \quad (4)$$

with

$$\begin{aligned} \psi(p, d) &= (k_{-5}\alpha(p, d), k_5p^2\alpha(p, d)) \\ \alpha(p, d) &= \frac{-k_4dp^2 + k_{-4}(c - d)}{k_{-4}(k_5p^2 + k_{-5})}. \end{aligned} \quad (5)$$

When $\varepsilon > 0$ is sufficiently small, numerical observations reveal the decay of fast transient motion as trajectories are attracted to a low-dimensional invariant set S_ε near S , as shown in Figure 1. Our objective is to approximate such invariant sets arbitrarily well.

1.1 Overview of the computational singular perturbation (CSP) method

Several algorithmic & computational techniques have been developed to identify these QSS (i.e. a lower dimensional slow manifold), and to identify the simplified system underlying long-term stability. Lam and Goussis [27, 28] devised the *computational singular perturbation* (CSP) method to identify reduced systems in chemical kinetics systems. The CSP method is an iterative procedure that generates a sequence of CSP manifolds and CSP fibers approximating the slow manifolds and fast fibers of the dynamical system; see Section 3 for details. The method has since been implemented with tremendous success for a variety of high-dimensional, nonstandard multiple-timescale problems, across combustion modelling, chemical reaction networks, and sensitive optimal control [30, 33, 37, 43, 44, 45]. To highlight just one representative example from the vast literature on numerical applications, CSP has been used in the numerical analysis of a combustion model to approximate a 12-dimensional invariant manifold in a 49-dimensional phase space of chemical species [33].

In a complementary direction, substantial theoretical progress has been made in understanding the convergence and geometrical content of the method. In 1995, Mease [35] used Fenichel theory as a framework to recast the CSP iteration step as a refinement of basis vectors which block-diagonalises the variational equations along trajectories lying in the slow invariant manifolds. Mease pointed out that the CSP method is equipped to deal with slow-fast systems beyond the standard form, using local coordinate transformations for the Fenichel normal form in his analysis.

In 2004-2005, Kaper, Kaper, and Zagaris proved convergence in a series of papers [16, 17] for slow-fast vector fields satisfying a spectral gap condition for the eigenvalues of the Jacobian of the vector field along an attracting invariant manifold, giving a rigorous proof for slow-fast systems in the standard form. In 2005, Valorani and his co-authors observed that the CSP iteration formulas may be decomposed into a eigenvector approximation scheme plus a piece that depends upon time derivatives of the Jacobian vector field [45]. By applying the chain rule, the latter terms are in turn related to second-derivatives of the Jacobian (with respect to the state space variables), and thus the CSP correction step inherently uses curvature (and higher-order geometrical characteristics) of the vector field in its computation. In 2015, Kaper, Kaper, and Zagaris [19] proved that the CSP iteration commutes with coordinate changes by taking advantage of the tensorial nature of the iteration. These results clarify that the rigorous convergence proofs given in their earlier papers do not in fact rely on the system being cast in the standard form, but rather only require local splittings of the tangent space along the critical manifold.²

²Mease also pointed out that the CSP method in principle should not even require the explicit identification of a small parameter ε . Rather, the CSP iteration should converge in powers of a uniform spectral gap over open sets in the phase space. Convergence proofs by Kaper, Kaper, and Zagaris [16, 17] refer to an explicit small parameter, and checking the spectral gap condition is an extremely challenging computational task in high-dimensional

We couch our current work in this more geometrical aspect of the literature. Our first goal is to write down refined CSP formulas for nonstandard slow-fast systems of the form

$$z' = H(z, \varepsilon) = N(z)f(z) + \varepsilon G(z, \varepsilon) \quad (6)$$

which includes systems with stoichiometric splittings of the form (1) as a sub-family. The idea is that the singular limit vector field factorization of (6), i.e. the vector field $h_0(z) := H(z, 0) = N(z)f(z)$, encodes a wealth of geometric information. Following the spirit of Mease's work, we assume the existence of a distinguished small parameter $\varepsilon > 0$ which characterises the ratio of slow and fast timescales, but we do not retreat to local coordinate representations or a Fenichel normal form. We instead revisit Fenichel's original, coordinate-independent framework. Our analysis culminates in Section 4.1 with a derivation of computable formulas for the first-order corrections of the slow manifold and fast fibers of the system in terms of the factorisation in (6).

Planar models of Michaelis-Menten chemical kinetics [15, 17], and the Davis-Skodje model [4, 19, 45] are popular low-dimensional examples in the standard form used to demonstrate the CSP step analytically, but there is a dearth of analytical examples for genuinely nonstandard problems. Part of the difficulty in the nonstandard case lies in the initialisation of the CSP iteration. Valorani [45] provided a numerical study of the convergence of the algorithm with respect to initialisations using eigenbases, standard unit vectors, and randomised unit vectors in two- and three-dimensional systems. Analytic computation of eigenvectors corresponding to slow and fast directions of point-dependent Jacobian matrices is difficult in all but the simplest cases. We show on the other hand that the factorisation in (6) provides a natural initialisation which further clarifies the CSP iteration (generally presented in terms of Jacobians and coordinate matrices), and is easier to compute algebraically. In the case of rational vector fields, this factorisation can often be read off from the form of $H(z, 0)$ or else computed using polynomial division algorithms from computational algebraic geometry [10]. Our second major goal is therefore to provide new analytically tractable, nonstandard examples of the CSP iteration. In Section 5 we apply these new techniques to a variety of nonstandard case studies of increasing dimension from two to four. The first three examples are planar problems of increasing complexity. The fourth is the aforementioned three-species kinetics problem derived in [45]. In this example we have the opportunity to augment their numerical analysis with new formulas for the first-order corrections of the relevant CSP objects. We finish with the four-dimensional slime cell model (3).

Although this paper is concerned with the CSP method, there are in fact a variety of iterative schemes to approximate invariant manifolds; the zero-derivative principle (ZDP) [8], intrinsic low-dimensional manifolds (ILDm) [31, 32], and center manifold normal-form reductions [39] are among a few of these (chapter 11 in [25] give an overview of the first three methods). Many of these

systems.

schemes are interconnected; for instance, the CSP and ZDP iterations differ only by a multiplicative factor [18].

The paper is organised as follows: In Sec. 2, we describe a general framework for nonstandard slow-fast systems. In Sec. 3 we define the two-step CSP update. Our main results are provided in Secs. 4 and 5: we give specific formulas for initializing the CSP method in the nonstandard context, study the output of the first update carefully, and then give examples demonstrating these formulas. We conclude in Sec. 6 by highlighting some fruitful new connections between the CSP method and the factorization given in the second section. We also provide an appendix (App. A), which expands on the framework underlying the CSP update step.

2 Nonstandard slow-fast dynamical systems

We begin by giving an abbreviated treatment of a general framework for nonstandard slow-fast systems. Much of this material in fact appears in Fenichel's seminal work on GSPT [7]; see also [36, 10]. This approach has been further developed by Wechselberger [47] and extends the framework to loss of normal hyperbolicity.

We are interested in two-timescale (or *slow-fast*) dynamical systems of the form (6), which we restate here for convenience:

$$z' = \frac{dz}{dt} = H(z, \varepsilon) = N(z)f(z) + \varepsilon G(z, \varepsilon), \quad (7)$$

with state variable $z \in \mathbb{R}^n$, $n \times (n - k)$ matrix $N(z)$ formed by column vectors $N^i(z) = (N_1^i(z), \dots, N_n^i(z))^T$ with sufficiently smooth functions $N^i : \mathbb{R}^n \rightarrow \mathbb{R}$, $i = 1, \dots, n - k$, $f(z) = (f_1(z), \dots, f_{n-k}(z))^T$ a column vector of sufficiently smooth functions $f_i : \mathbb{R}^n \rightarrow \mathbb{R}$, $i = 1, \dots, n - k$, $G(z, \varepsilon) = (G_1(z, \varepsilon), \dots, G_n(z, \varepsilon))^T$ a column vector of sufficiently smooth functions $G_i : \mathbb{R}^n \rightarrow \mathbb{R}$, $i = 1, \dots, n$, and $\varepsilon \ll 1$ characterizes the ratio of timescales in the system.

Definition 2.1 *Let S_0 denote the set of equilibria of system (7) in the singular limit $\varepsilon \rightarrow 0$. If there exists a subset $S \subseteq S_0$ which forms a k -dimensional differentiable manifold of equilibria with $1 \leq k < n$, then system (7) defines a singular perturbation problem.*

Assumption 2.1 *System (7) is a singular perturbation problem with a single subset $S \subseteq S_0$,*

$$S = \{z \in \mathbb{R}^n : f(z) = 0\}, \quad (8)$$

which forms a k -dimensional differentiable manifold of equilibria, $1 \leq k < n$, called the critical manifold.

Assumption 2.2 *In system (7), the matrix $N(z)$ has full (column) rank for all $z \in S$.*

Next consider system (7), rescaled from the fast timescale t to the slow timescale $\tau = \varepsilon t$:

$$\dot{z} = \frac{dz}{d\tau} = \frac{1}{\varepsilon}H(z, \varepsilon) = \frac{1}{\varepsilon}N(z)f(z) + G(z, \varepsilon), \quad (9)$$

Systems (7) and (9) are equivalent when $\varepsilon > 0$ but their singular limits $\varepsilon \rightarrow 0$ are not. In fact, they carry complementary, lower dimensional information, and it is a cornerstone of GSPT to *concatenate* the information from these two limiting problems to deduce the dynamics of the full system (7) respectively (9).

2.1 The layer problem

We focus first on system (7) evolving on the fast time scale t .

Definition 2.2 *The layer problem of system (7) is given by the formal limit $\varepsilon \rightarrow 0$:*

$$z' = H(z, 0) = N(z)f(z). \quad (10)$$

Under Assumption 2.1, the set S forms a k -dimensional manifold of equilibria of the layer problem. Hence, the Jacobian $Dh|_S$ along S has k *trivial* zero eigenvalues and $(n - k)$ *nontrivial* eigenvalues.

Definition 2.3 *A k -dimensional critical manifold S is called normally hyperbolic if the $(n - k)$ nontrivial eigenvalues of the Jacobian $Dh|_S = (NDf)|_S$ are bounded away from the imaginary axis.*

The existence of a normally hyperbolic manifold implies the following splitting:

$$T_z\mathbb{R}^n = T_zS \oplus \mathcal{N}_z, \quad \forall z \in S \quad (11)$$

where T_zS denotes the tangent space of the critical manifold S at z , coinciding with the kernel of the linear map $DH(z, 0)$, and \mathcal{N}_z is the unique complement of the splitting identified with the quotient space $T_z\mathbb{R}^n/T_zS$. We call \mathcal{N}_z the *linear fast fiber with basepoint $z \in S$* . Repeating this construction across all points of S , we obtain the tangent bundle $TS = \cup_{z \in S} T_zS$ of S , and the transverse linear fast fiber bundle $\mathcal{N} = \cup_{z \in S} \mathcal{N}_z$. This splitting induces unique projection operators onto the tangent bundle TS and the linear fast fibre bundle \mathcal{N} as follows:

$$\Pi^S : TS \oplus \mathcal{N} \rightarrow TS. \quad (12)$$

$$\Pi^N : TS \oplus \mathcal{N} \rightarrow \mathcal{N} = I - \Pi^S. \quad (13)$$

Lemma 1 *At any point $z \in S$ of a normally hyperbolic manifold S , the rows of $Df(z)$ form a basis of $T_z S^\perp$ and the columns of $N(z)$ form a basis of \mathcal{N}_z .*

Proof. The manifold S is the zero level set of $f(z)$ which forms a k -dimensional manifold, i.e. $Df(z)|_S$ has full row rank $(n - k)$ for any $z \in S$. Thus the rows of $Df(z)$ form a basis of the orthogonal complement of $T_z S$.

Since S is normally hyperbolic, we have $DH(z, 0)$ has rank $(n - k)$ which implies $\ker DH(z, 0) = T_z S$ at points $z \in S$. Under Assumption 2.2, $N(z)$ has full column rank $(n - k)$. Thus the column spaces of $DH(z, 0)$ and $N(z)$ coincide at points $z \in S$ and, hence, the columns of $N(z)$ form a basis of \mathcal{N}_z . \square

Lemma 2 *Let S be a normally hyperbolic manifold. Then the $(n - k) \times (n - k)$ square matrix $DfN|_S$ is regular, and its eigenvalues are equal to the set of nontrivial eigenvalues of $Dh|_S$.*

Proof. Let the linear operator $DH(z, 0)|_S$ act on the basis of the invariant subset \mathcal{N} , i.e.

$$DH(z, 0)N(z)|_S = (N(z)Df(z))N(z)|_S = N(z)(Df(z)N(z))|_S.$$

By Lemma 1, the $(n - k) \times (n - k)$ square matrix $DfN|_S$ is necessarily a regular matrix with $(n - k)$ nonzero eigenvalues which coincide with the nontrivial eigenvalues of $DH(z, 0)|_S$. Note, if $p(z) \in \mathbb{R}^{n-k}$ is an eigenvector of $DfN|_S$ with eigenvalue $\mu(z)$ then $N(z)p(z) \in \mathbb{R}^n$ is the corresponding eigenvector of $DH(z, 0)$ with the same eigenvalue. \square

Assumption 2.3 *The k -dimensional critical manifold S of system (7) is normally hyperbolic and attracting, i.e. all $(n - k)$ nontrivial eigenvalues have negative real part.*

Remark 1 *System (3) satisfies Assumptions 2.1–2.3. A rich source of examples comes from chemical reaction networks; Schauer and Heinrich [40] provide a derivation of such models with the goal of identifying quasi-steady state approximations in biochemical reaction networks.*

Nevertheless, it is unclear whether general techniques exist to compute such factorizations in a typical slow-fast system. In the case of polynomial vector fields, Goeke and Walcher [10] have used division algorithms for algebraic varieties to factor $H(z, 0)$.

Remark 2 *In this paper we do not concern ourselves with singularities of $H(z, 0)$ outside of the critical manifold S ; we only require the local geometric*

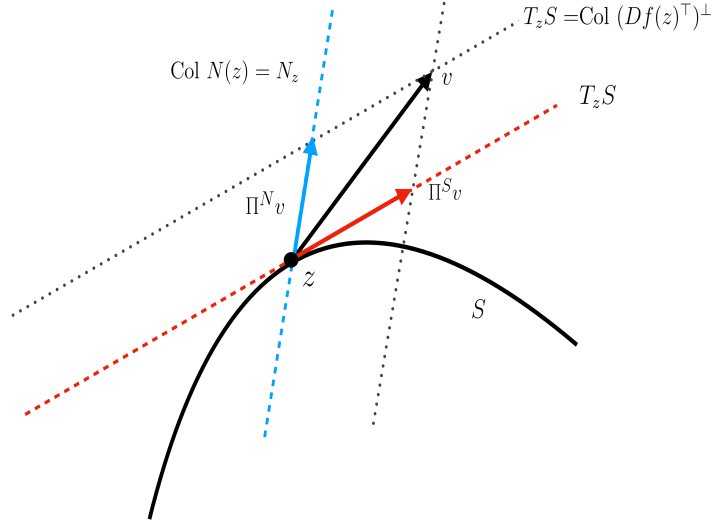


Figure 2: A sketch of the projectors Π^S (12) and Π^N (13) defined at a point $z \in S$. The invariant subspaces $T_z S$ and N_z are illustrated by red and blue dashed lines, respectively, together with an arbitrary vector $v \in T_z \mathbb{R}^n$. The dotted lines are parallel translates of these subspaces along the oblique projections $\Pi^S v$ and $\Pi^N v$.

structure provided by the differentiable manifold and transverse fibers in the preceding arguments. A simple example of a system having an isolated singularity as well as a critical manifold is given in Sec. 5.1.

2.2 The reduced problem

Now consider system (9) evolving on the slow timescale $\tau = \varepsilon t$. The singular limit $\varepsilon \rightarrow 0$ of system (9) requires more care, i.e. this limit will only be well-defined provided that we restrict the phase space to S and that $G(z, 0)$ is restricted to the tangent bundle TS . The projection operator Π^S (12) allows us to formulate this limit.

Definition 2.4 *The reduced problem of system (9) is*

$$\dot{z} = \frac{d}{d\tau} z = \Pi^S \left. \frac{\partial}{\partial \varepsilon} H(z, \varepsilon) \right|_{\varepsilon=0} = \Pi^S G(z, 0). \quad (14)$$

Definition 2.5 Consider the splitting $\mathbb{R}^n = \mathcal{V} \oplus \mathcal{W}$, where \mathcal{V} has dimension $n - k$ and \mathcal{W} has dimension k . The oblique projection of a vector $p = x + y$, $x \in \mathcal{V}$ and $y \in \mathcal{W}$, onto the subspace \mathcal{V} parallel to \mathcal{W} is a linear map $\Pi^{\mathcal{V}} = (\Pi^{\mathcal{V}})^2$ satisfying $\Pi^{\mathcal{V}}(p) = x$.

Suppose V (resp. U) is an $n \times (n - k)$ matrix whose column vectors span \mathcal{V} (resp. \mathcal{W}^\perp). Then it can be shown that $\Pi^{\mathcal{V}}$ has the following matrix representation:

$$\Pi^{\mathcal{V}} = V(U^\top V)^{-1}U^\top. \quad (15)$$

The (complementary) oblique projection onto the subspace \mathcal{W} parallel to \mathcal{V} is given by

$$\Pi^{\mathcal{W}} = I - \Pi^{\mathcal{V}}. \quad (16)$$

In the present context, the splitting $T\mathbb{R}^n = \mathcal{N} \oplus TS$ induces an oblique projection onto the tangent bundle of the critical manifold, parallel to the fast fibers (see Fig. 2). Lemma 1 gives us a matrix representation using the matrices N and Df :

$$\Pi^S = I - N(DfN)^{-1}Df. \quad (17)$$

The complementary oblique projection onto the fast fibers is denoted $\Pi^N := I - \Pi^S$. By Lemma 2, the matrix DfN is regular and, hence, the inverse is well defined. Equivalent projection formulas appear in [7] and [10].

Remark 3 It is easily shown that standard singular perturbation problems are a special case of a nonstandard problem (7). Indeed, select

$$N = \begin{pmatrix} \mathbb{O}_{k,n-k} \\ \mathbb{I}_{n-k,n-k} \end{pmatrix} \quad (18)$$

and describe the variables and vector field in terms of components $z = (x, y) \in \mathbb{R}^k \times \mathbb{R}^{(n-k)}$ and $G(x, y, \varepsilon) = (g(x, y, \varepsilon), \tilde{f}(x, y, \varepsilon))$. Then $z' = N(z)f(z) + \varepsilon G(z, \varepsilon)$ gives

$$\begin{aligned} x' &= \varepsilon g(x, y, \varepsilon) \\ y' &= f(x, y, \varepsilon) + \varepsilon \tilde{f}(x, y, \varepsilon), \end{aligned} \quad (19)$$

which is a standard singular perturbation problem. From (19) we observe that x lists the k slow variables and y lists the $(n - k)$ fast variables. These systems lie in contrast to the nonstandard case, where one cannot expect such a trivial factorization (18) to exist globally.

2.3 Fenichel Theory

In the case of normally hyperbolic critical manifolds, QSS reductions onto a slow invariant manifold are justified by the following theorem.

Theorem 1 (Fenichel's Theorem [7, 14, 25]) *Given the system (7) with a C^r -smooth vector field and a compact normally hyperbolic critical manifold, the following hold for $\varepsilon > 0$ sufficiently small:*

- *There exists a locally invariant C^r -smooth, normally hyperbolic slow manifold S_ε that is C^r $\mathcal{O}(\varepsilon)$ -close to S .*
- *The flow on S_ε converges to the reduced flow on S as $\varepsilon \rightarrow 0$.*
- *There are C^r -smooth locally invariant stable and unstable manifolds, $\mathcal{F}^s(S_\varepsilon)$ and $\mathcal{F}^u(S_\varepsilon)$.*
- *These manifolds admit nonlinear, C^{r-1} -smooth foliations $\{\mathcal{F}^s(p) : p \in S_\varepsilon\}$ resp. $\{\mathcal{F}^u(p) : p \in S_\varepsilon\}$. Furthermore, these families are positively (resp. negatively) invariant on fibers; i.e. if ϕ_t is the time- $t \geq 0$ flow map of (7) and if $p, \phi_t(p) \in S_\varepsilon$, then*

$$\phi_t(\mathcal{F}^s(p)) \subseteq \mathcal{F}^s(\phi_t(p)).$$

An analogous statement holds for the fibers $\mathcal{F}^u(p)$, with $p \in S_\varepsilon$.

- *There exist constants $C, \lambda > 0$ such that if $q \in \mathcal{F}^s(p)$, then for $t \geq 0$ we have*

$$\|\phi_t(p) - \phi_t(q)\| < Ce^{-\lambda t}.$$

Analogous rate estimates hold for the fibers $\mathcal{F}^u(p)$, with $p \in S_\varepsilon$.

The invariant slow manifold S_ε and its invariant nonlinear foliation \mathcal{F}_ε (which split into the sub-foliations given in the theorem above) organise the dynamics of the full system: trajectories perturb from concatenated orbits of the layer and reduced problems under the appropriate transversality conditions. In analogy to the $\varepsilon = 0$ setting, we denote the linear fast fiber at basepoint $p \in S_\varepsilon$ by $\mathcal{N}_{\varepsilon,p}$ and the linear fast fiber bundle by $\mathcal{N}_\varepsilon = \cup_{p \in S_\varepsilon} \mathcal{N}_{\varepsilon,p}$.

3 The CSP iteration

Suppose that the invariant slow manifold S_ε of a nonstandard slow-fast system (7) is (locally) given by the graph of a function $y = h_\varepsilon(x)$ with $h_\varepsilon : \mathbb{R}^k \rightarrow \mathbb{R}^{n-k}$. We express $h_\varepsilon(x)$ as an asymptotic series in ε :

$$y = h_\varepsilon(x) = h_0(x) + \varepsilon h_1(x) + \varepsilon^2 h_2(x) + \cdots + \varepsilon^j h_j(x) + \mathcal{O}(\varepsilon^{j+1}). \quad (20)$$

The terms $h_j(x)$ may be obtained reinserting this series into (7) and matching coefficients in orders of ε . The CSP method adopts a different, iterative approach to efficiently compute not only the terms $h_j(x)$, but also a similar asymptotic approximation to the linear fast fibers transverse to the slow manifold. The motivating idea is to understand how the variational equation of a dynamical system is affected by changes in basis.

3.1 Geometric framework of the CSP method

Consider a smooth vector field $H(z)$, to which we append the variational equation to produce the dynamical system on the tangent bundle:

$$\begin{aligned} z' &= H(z) \\ H' &= DH(z)H(z). \end{aligned} \quad (21)$$

Under some arbitrarily chosen splitting $z = (x, y)$, where $x \in \mathbb{R}^{n-k}$ and $y \in \mathbb{R}^k$, we can write the variational equation in block component form:

$$\begin{pmatrix} H'_x \\ H'_y \end{pmatrix} = \begin{pmatrix} D_x H_x & D_y H_x \\ D_x H_y & D_y H_y \end{pmatrix} \begin{pmatrix} H_x \\ H_y \end{pmatrix}. \quad (22)$$

Now suppose $A(z) = [A_f(z) \ A_s(z)]$ is a smooth, regular $n \times n$ matrix for all $z \in S$ with $B(z) = \begin{pmatrix} B_{s\perp}(z) \\ B_{f\perp}(z) \end{pmatrix}$ its dual. Here, the first and second block columns of A , denoted A_f and A_s , are of sizes $n \times (n-k)$ and $n \times k$, respectively; similarly, the first and second block rows $B_{s\perp}$ and $B_{f\perp}$ have sizes $(n-k) \times n$ and $k \times n$, respectively. The vector field $H(z)$ expressed in this new basis is given by

$$g(z) = B(z)H(z). \quad (23)$$

Definition 3.1 For a smooth $n \times m$ matrix function X and a smooth vector field H , $[X, H]$ is denoted the Lie bracket of X and H and defined as the $n \times m$ matrix whose i th column is

$$\begin{aligned} [X, H]_i &= [X_i, H] \\ &= (DH)X_i - (DX_i)H, \end{aligned}$$

where $i = 1, \dots, m$ and A_i refers to the i th column of A .

It can be shown that the variational equation of the transformed vector field can be written compactly in the form

$$g' = \Lambda(A, B, H)g, \quad (24)$$

where the nonlinear operator $\Lambda(A, B, H)$ has the algebraic structure of a Lie bracket:

$$\Lambda(A, B, H) = B[A, H]; \quad (25)$$

see the appendix (Sec. A.1) for a derivation of this result. The operator Λ can be written in block-component form:

$$\Lambda = \begin{pmatrix} \Lambda_{ff} & \Lambda_{fs} \\ \Lambda_{sf} & \Lambda_{ss} \end{pmatrix} = \begin{pmatrix} B_{s\perp}[A_f, H] & B_{s\perp}[A_s, H] \\ B_{f\perp}[A_f, H] & B_{f\perp}[A_s, H] \end{pmatrix}. \quad (26)$$

The key insight is that in the presence of a k -dimensional invariant manifold \mathcal{M} and corresponding transverse linear fiber bundle \mathcal{N} , the vector field H may be expressed in a clever choice of basis $A(z)$ and dual $B(z)$ which block-diagonalizes Λ . As a consequence, the invariant manifold \mathcal{M} and the linear fiber bundle \mathcal{N} are easily characterized in terms of this basis as follows:

$$\mathcal{M} = \{z \in \mathbb{R}^n : B_{s\perp}(z)H(z) = 0\}, \quad (27)$$

$$\mathcal{N} = \bigcup_{p \in \mathcal{M}} \mathcal{N}_p = \bigcup_{p \in \mathcal{M}} \text{Col}(A_f(p)); \quad (28)$$

see the appendix (Sec. A.2) for details. This formalism applies directly to the case of an invariant slow manifold $\mathcal{M} = S_\varepsilon$ and its accompanying linear fast fiber bundle $\mathcal{N} = \mathcal{N}_\varepsilon$, as defined by Fenichel's theorem (Sec. 2.3). The characterizations (27)–(28) then state that S_ε is defined by the locus of points $B_{s\perp}(z)H(z) = 0$ where the components of the vector field $H(z)$ lying in the direction of the linear fast fibers vanish, and that the linear fast fibers \mathcal{N}_p at basepoints $p \in S_\varepsilon$ are spanned by the columns of the block component $A_f(p)$.

3.2 CSP objects

The CSP iteration acts on a suitably initialised (point-dependent) basis matrix $A^{(0)}(z)$ and dual $B^{(0)}(z)$, producing a sequence $\{(A^{(j)}(z), B^{(j)}(z))\}_{j=0}^\infty$ of successively refined bases. We initialise with the pair

$$\begin{aligned} A^{(0)} &= \begin{pmatrix} A_f^{(0)} & A_s^{(0)} \end{pmatrix} \\ B^{(0)} &= \begin{pmatrix} B_{s\perp}^{(0)} \\ B_{f\perp}^{(0)} \end{pmatrix}. \end{aligned} \quad (29)$$

The sequence $\{(A^{(j)}(z), B^{(j)}(z))\}_{j=0}^\infty$ in turn defines a sequence of updates $\{\Lambda^{(j)}\}_{j=0}^\infty$ to the Λ operator:

$$\Lambda^{(j)} = B^{(j)}[A^{(j)}, H]. \quad (30)$$

These approximate operators may be written in block components in analogy to (26). Motivated by the characterizations of the invariant manifold and fast fibers provided in Eqs. (27)–(28), we define the following approximating objects:

Definition 3.2 *The CSP manifold of order 0 is the level set*

$$\mathcal{K}^{(0)} = \{(x, y) \in \mathbb{R}^n : B_{s\perp}^{(0)}(x, y, \varepsilon)H(x, y, \varepsilon) = \mathbb{O}_{n-k,1}\}. \quad (31)$$

For integers $j \geq 1$, the CSP manifold of order j , denoted $\mathcal{K}^{(j)}$, is

$$\mathcal{K}^{(j)} = \{(x, y) \in \mathbb{R}^n : B_{s\perp}^{(j)}(x, \psi^{(j-1)}(x, \varepsilon), \varepsilon)H(x, y, \varepsilon) = \mathbb{O}_{n-k,1}\}, \quad (32)$$

where $y = \psi^{(j-1)}(x, \varepsilon)$ is a graph of $\mathcal{K}^{(j-1)}$.

Definition 3.3 For $j \geq 0$ and $p \in \mathcal{K}^{(j)}$, the CSP fiber of order j is the subspace

$$\mathcal{L}^{(j)}(p) = \text{Col } A_f^{(j)}(p, \varepsilon). \quad (33)$$

The CSP fiber bundle of order j is the corresponding vector bundle

$$\mathcal{L}^{(j)} = \bigcup_{p \in \mathcal{K}^{(j)}} \mathcal{L}_\varepsilon^{(j)}(p). \quad (34)$$

Remark 4 The convergence of the CSP manifolds and fiber bundles to the invariant slow manifold and fast fiber bundle of system (7) depends on the choice of iteration step, as shown in Sec. 3.4.

3.3 One-step and two-step CSP updates

There are two commonly-used variants of the CSP iteration. We will only apply the two-step method in this paper, but it is instructive to introduce the simpler one-step method to clarify the relationship between these iterations and the CSP objects (32)–(33).

Both methods use near-identity transformations in the update step, i.e. multiplication by matrices of the form $I \pm U$ and $I \pm L$, where I is the identity matrix, and U and L are nilpotent matrices of the form

$$\begin{aligned} U^{(j)} &= \begin{pmatrix} \mathbb{O}_{n-k, n-k} & \tilde{U}^{(j)} \\ \mathbb{O}_{k, n-k} & \mathbb{O}_{k, k} \end{pmatrix} \\ L^{(j)} &= \begin{pmatrix} \mathbb{O}_{n-k, n-k} & \mathbb{O}_{n-k, k} \\ \tilde{L}^{(j)} & \mathbb{O}_{k, k} \end{pmatrix}. \end{aligned} \quad (35)$$

The block components $\tilde{U}^{(j)}$ and $\tilde{L}^{(j)}$, of respective sizes $(n-k) \times k$ and $k \times (n-k)$, are defined by the constraint that the CSP manifolds and fibers converge asymptotically to the slow manifold and linear fast fibers; see Sec. 3.4. Near-identity update matrices are computationally easy to invert. In particular, we obtain efficient update rules for the dual basis $B^{(j)}$, as shown in the following two methods.

3.3.1 One-step CSP method

The one-step CSP method is given by the iteration rule

$$\begin{aligned} A^{(j+1)} &= A^{(j)}(I - U^{(j)}) = \begin{pmatrix} A_f^{(j)} & A_s^{(j)} - A_f^{(j)} \tilde{U}^{(j)} \end{pmatrix} \\ B^{(j+1)} &= (I + U^{(j)})B^{(j)} = \begin{pmatrix} B_{s\perp}^{(j)} + \tilde{L}^{(j)} B_{f\perp}^{(j)} \\ B_{f\perp}^{(j)} \end{pmatrix}. \end{aligned} \quad (36)$$

The one-step CSP method only updates ‘half’ of the basis. This update is sufficient if we are interested in computing only the CSP manifolds (32). If we wish to approximate the fast fibers to the invariant manifold in tandem, we must update the remaining blocks of the basis and dual basis matrices. This update is provided by the two-step CSP method.

3.3.2 Two-step CSP method

The two-step CSP method is given by the iteration rule

$$\begin{aligned}
 A^{(j+1)} &= A^{(j)}(I - U^{(j)})(I + L^{(j)}) \\
 &= \begin{pmatrix} A_f^{(j)}(I - \tilde{U}^{(j)}\tilde{L}^{(j)}) + A_s^{(j)}\tilde{L}^{(j)} & A_s^{(j)} - A_f^{(j)}\tilde{U}^{(j)} \end{pmatrix} \\
 B^{(j+1)} &= (I - L^{(j)})(I + U^{(j)})B^{(j)}, \\
 &= \begin{pmatrix} B_{s\perp}^{(j)} + \tilde{U}^{(j)}B_{f\perp}^{(j)} \\ (I - \tilde{L}^{(j)}\tilde{U}^{(j)})B_{f\perp}^{(j)} - \tilde{L}^{(j)}B_{s\perp}^{(j)} \end{pmatrix}.
 \end{aligned} \tag{37}$$

3.4 Convergence

Suppose that after j iterates of the CSP two-step method, the CSP manifold of order j defined by (32) is locally expressed as a graph $y = \psi^{(j)}(x, \varepsilon)$ and then expanded as an asymptotic series in ε :

$$y = \psi^{(j)}(x, \varepsilon) = \psi_0^{(j)}(x) + \varepsilon\psi_1^{(j)}(x) + \varepsilon^2\psi_2^{(j)}(x) + \dots \tag{38}$$

When the update terms in the near-identity transformations (37) are defined appropriately, Kaper, Kaper, and Zagaris [16] demonstrated convergence of the CSP manifold to the invariant slow manifold of Fenichel’s theory (as described in Sec. 2.3), in the following sense.

Theorem 2 (Convergence of CSP manifolds [16]) *Suppose the leading-order term of the graph of $\mathcal{K}^{(0)}$, denoted $y = \psi^{(0)}(x, \varepsilon)$, agrees with the graph of the critical manifold $y = h_0(x)$ under a local choice of coordinates. Then using the one-step or two-step CSP update rule and for j fixed, we have*

$$y = \psi^{(j)}(x, \varepsilon) = \sum_{i=0}^j \varepsilon^i h_i(x) + \mathcal{O}(\varepsilon^{j+1})$$

when $\varepsilon > 0$ is sufficiently small, where $\psi^{(j)}$ is the graph of $\mathcal{K}^{(j)}$ with asymptotic series expansion (38) and $y = h(x) = \sum_{j=0}^{\infty} h_j(x)$ is the asymptotic series expansion of the graph of S_ε .

This theorem states if the CSP two-step method is initialised appropriately, then for pairs of indices $0 \leq i \leq j$ we have $\psi_i^{(j)}(x) = h_i(x)$. This justifies the

nomenclature ‘CSP manifold of order j ’: the set $\mathcal{K}^{(j)}$ agrees with S_ε up to order j terms in the asymptotic expansion.

An analogous convergence statement can be given for the CSP fiber bundle (34):

Theorem 3 (Convergence of CSP fibers [17]) *Fix $j \geq 0$ and let $\mathcal{K}^{(j)}$ be given locally by the graph $y = \psi^{(j)}(x)$ for $x \in \mathbb{R}^k$ and $y \in \mathbb{R}^{n-k}$. Then given the basepoint $(x, \psi^{(j)}(x))$ on $\mathcal{K}^{(j)}$ (resp. $(x, h_\varepsilon(x))$ on S_ε), the asymptotic expansions of $\mathcal{L}^{(j)}(x, \psi^{(j)}(x))$ (as defined in (33)) and $N_\varepsilon(x, h(x))$ agree up to and including terms of $\mathcal{O}(\varepsilon^j)$. Thus, the CSP fast fiber bundle $\mathcal{L}^{(j)}$ is an $\mathcal{O}(\varepsilon^j)$ approximation to the fast fiber bundle N_ε .*

Theorems 2–3 hold when the near-identity updates in (35) are defined as follows:

$$\begin{aligned}\tilde{U}^{(j)} &= (\Lambda_{ff}^{(j)})^{-1} \Lambda_{fs}^{(j)} \\ \tilde{L}^{(j)} &= \Lambda_{sf}^{(j)} (\Lambda_{ff}^{(j)})^{-1}.\end{aligned}\tag{39}$$

With this choice of update step, the CSP two-step method simultaneously block-diagonalizes the CSP operator $\Lambda^{(j)}$ (as defined in (30)) in discrete steps as follows [17]:

Lemma 3 *For $j = 0, 1, \dots$, the CSP two-step method (37) provides the asymptotic estimates*

$$\Lambda^{(j)} = \begin{pmatrix} \Lambda_{ff,0} + \mathcal{O}(\varepsilon) & \mathcal{O}(\varepsilon^j) \\ \mathcal{O}(\varepsilon^j) & \mathcal{O}(\varepsilon) \end{pmatrix},$$

where $\Lambda^{(j)}$ is evaluated on $\mathcal{K}^{(j)}$.

4 Nonstandard CSP updates

We remind the reader that rigorous convergence proofs for the standard form are provided in [16, 17], and the CSP iteration commutes with coordinate changes [19]. We can now proceed to describe the CSP update step for nonstandard slow-fast systems (7) satisfying Assumptions 2.1–2.3. The key is that bases for the fast and slow subspaces can be ‘read off’ using the factorization $H(z, 0) = N(z)f(z)$, providing a natural initial condition for the iteration. By Lemma 1, the columns of $N(z)$ span the linear fast fiber with basepoint $z \in S$, and the columns of $Df(z)^\top$ span $T_z S^\perp$. Thus,

$$A^{(0)} = (N \quad (Df^\top)^\perp)\tag{40a}$$

$$B^{(0)} = \begin{pmatrix} Q_1 Df \\ Q_2 (N^\perp)^\top \end{pmatrix},\tag{40b}$$

where the notation P^\perp refers to a matrix whose columns form a basis to the subspace orthogonal to the column space of the matrix P , and the regular prefactors

$$\begin{aligned} Q_1 &= (DfN)^{-1} \\ Q_2 &= ((N^\perp)^\top (Df^\top)^\perp)^{-1} \end{aligned} \quad (41)$$

in the block rows (which are well-defined by Lemma 1) have been selected to normalize the block diagonal components in the product $B^{(0)}A^{(0)}$ to the identity. With this initialization, the leading-order approximation $\mathcal{K}^{(0)}$ of the CSP manifold defined in (31) can be computed:

$$\begin{aligned} B_{s\perp}^{(0)}H &= 0 \\ (DfN)^{-1}Df(Nf + \varepsilon G) &= 0 \\ f + \varepsilon(DfN)^{-1}(DfG) &= 0 \\ f &= -\varepsilon(DfN)^{-1}(DfG). \end{aligned} \quad (42)$$

This level set implicitly defines the graph $y = \psi^{(0)}(x, \varepsilon)$. On this graph, we expand both sides of this equation in powers of ε . The leading-order $O(\varepsilon^0)$ coefficient is

$$f(x, \psi_0(x), 0) = 0, \quad (43)$$

which matches the definition of the critical manifold S as the leading-order part of the asymptotic series of \mathcal{S}_ε , $f(x, h_0(x), 0) = 0$; thus, $\psi_0^{(0)}(x) = h_0(x)$.

The four block components of the operator $\Lambda^{(0)} = B^{(0)}[A^{(0)}, H]$ can be computed explicitly in terms of the components N , f , and G in the vector field H . We list them compactly (compare with (26)):

$$\Lambda_{ff}^{(0)} = DfN + \varepsilon Q_1 Df[N, G] \quad (44a)$$

$$\Lambda_{fs}^{(0)} = \varepsilon Q_1 Df([(Df^\top)^\perp, G] - [(Df^\top)^\perp, N]Q_1 DfG) \quad (44b)$$

$$\Lambda_{sf}^{(0)} = \varepsilon Q_2 (N^\perp)^\top [N, G] \quad (44c)$$

$$\Lambda_{ss}^{(0)} = \varepsilon Q_2 (N^\perp)^\top ([(Df^\top)^\perp, G] - [(Df^\top)^\perp, N]Q_1 DfG). \quad (44d)$$

The tensorial nature of the CSP update step was identified and explored in [19]. In our setting, tensor properties of some of the terms such as DN play a significant role in simplifying the formulas for $\Lambda^{(0)}$. These calculations are presented in the Appendix A.3.

The vector function f is $\mathcal{O}(\varepsilon)$ on $\mathcal{K}^{(0)}$ by (42); therefore, the latter three block components are at most $\mathcal{O}(\varepsilon)$ as well. This in turn implies that the update blocks $\tilde{U}^{(0)}$ and $\tilde{L}^{(0)}$ defined in (39) are both $\mathcal{O}(\varepsilon)$ on this set. After one application of the CSP two-step update (37), the updated bases $A^{(1)}$ and $B^{(1)}$

are

$$A^{(1)} = \left(A_f^{(0)} + A_s^{(0)} \tilde{L}^{(0)} - A_f^{(0)} \tilde{U}^{(0)} \tilde{L}^{(0)} \quad -A_f^{(0)} \tilde{U}^{(0)} + A_s^{(0)} \right) \quad (45a)$$

$$B^{(1)} = \begin{pmatrix} B_{s\perp}^{(0)} + \tilde{U}^{(0)} B_{f\perp}^{(0)} \\ B_{f\perp}^{(0)} - \tilde{L}^{(0)} B_{s\perp}^{(0)} - \tilde{L}^{(0)} \tilde{U}^{(0)} B_{f\perp}^{(0)} \end{pmatrix}. \quad (45b)$$

The block components $\tilde{L}^{(0)}$ and $\tilde{U}^{(0)}$ each introduce $\mathcal{O}(\varepsilon^1)$ perturbations of the initial block columns of $A^{(0)}$ (respectively block rows of $B^{(0)}$).

4.1 First-order corrections of the slow manifold and fast fibers

We now demonstrate the computability of the CSP formulas with the following two lemmas, which give new formulas for the first-order corrections of S_ε and \mathcal{N}_ε , respectively.

Lemma 4 *Assume the conditions of Fenichel's theorem (Theorem 1) are satisfied for a sufficiently smooth family of vector fields of the form (7), and suppose the slow manifold S_ε is written locally as a graph*

$$y = h(x, \varepsilon) = h_0(x) + \varepsilon h_1(x) + \mathcal{O}(\varepsilon^2)$$

with $D_y f|_S$ having full rank. Then the first-order correction term is given by the computable formula

$$h_1(x) = -(D_y f)^{-1} (DfN)^{-1} (DfG) \quad (46)$$

when $\varepsilon > 0$ is sufficiently small.

Proof. Our objective is to compute the $\psi_1^{(1)}$ term of the first CSP update in terms of N, f , and G . The Theorem 2 allows us to equate this term with the first-order correction of the asymptotic expansion of S_ε . The first update of the CSP manifold $\mathcal{K}^{(1)}$ is defined as follows; see (32):

$$\begin{aligned} B_{s\perp}^{(1)}(x, \psi^{(0)}(x, \varepsilon), \varepsilon) H(x, y, \varepsilon) &= 0 \\ (Df_0 N_0)^{-1} Df_0 (Nf + \varepsilon G) + \Lambda_{ff,0}^{-1} \Lambda_{fs,0} B_{f\perp,0} (Nf + \varepsilon G) &= 0. \end{aligned}$$

In this equation and the following, we use the additional subscript '0' to refer to those quantities that are computed on points $(x, \psi^{(0)}(x)) \in \mathcal{K}^{(0)}$. We compute the order $\mathcal{O}(\varepsilon^1)$ coefficient of the asymptotic series assuming the graph form $y = \psi^{(1)}(x, \varepsilon)$ where the leading order coefficient is defined by $f_0 = 0$; see (43):

$$\begin{aligned} (Df_0 N_0)^{-1} Df_0 (N_0 f_0 + \varepsilon (N_0 D_y f_0 \psi_1^{(1)} + G_0)) + \\ \Lambda_{ff,0}^{-1} \Lambda_{fs,0} B_{f\perp,0} (N_0 f_0 + \varepsilon (N_0 D_y f_0 \psi_1^{(1)} + G_0)) + \mathcal{O}(\varepsilon^2) &= 0. \end{aligned}$$

We first evaluate the asymptotics of the second line. We have

$$\begin{aligned}\Lambda_{ff,0}^{-1} &= (Df_0N_0)^{-1} + \mathcal{O}(\varepsilon) \\ \Lambda_{fs,0} &= \mathcal{O}(\varepsilon) \\ N_0f_0 + \varepsilon(N_0D_yf_0\psi_1^{(1)} + G_0) &= -\varepsilon N_0(Df_0N_0)^{-1}Df_0G_0 + \varepsilon(N_0D_yf_0\psi_1^{(1)} + G_0) \\ &= \mathcal{O}(\varepsilon).\end{aligned}$$

Therefore, the second line is at most $\mathcal{O}(\varepsilon^2)$ on $\mathcal{K}^{(0)}$. The remaining $\mathcal{O}(\varepsilon^1)$ terms give

$$\begin{aligned}\varepsilon D_y f_0 \psi_1^{(1)} + \varepsilon (Df_0 N_0)^{-1} Df_0 G_0 &= 0 \\ \psi_1^{(1)} &= -(D_y f_0)^{-1} (Df_0 N_0)^{-1} (Df_0 G_0).\end{aligned}$$

By Theorem 2, $\psi_1^{(1)} = h_1$. \square

Remark 5 *This result matches a recent result due to Wechselberger [47] for the first-order correction of \mathcal{S}_ε in the nonstandard case.*

Lemma 5 *Assume the conditions for Fenichel's theorem (1) are satisfied for a sufficiently smooth family of vector fields of the form (7), so that the linear fast fiber $\mathcal{N}_\varepsilon(x, h_\varepsilon(x))$ at basepoint $(x, h_\varepsilon(x)) \in S_\varepsilon$ admits a local expansion as an asymptotic series of the form*

$$\mathcal{N}_\varepsilon(x, h_\varepsilon(x)) = \text{span}(k_0(x) + \varepsilon k_1(x) + \mathcal{O}(\varepsilon^2)).$$

Then $k_0(x) = N(x, h_0(x))$ and

$$k_1(x) = \Pi^S[N, G](DfN)^{-1}. \quad (47)$$

Proof. In analogy to the previous lemma, we take advantage of the convergence of the CSP iteration to produce a formula for the CSP fiber of order one, and then we apply a slightly stronger variant of the convergence theorem for linear fast fibers (Theorem 3). Let $\mathcal{L}^{(1)} = \text{Col}(A_f^{(1)})$, defined by (37). We have

$$\begin{aligned}A_f^{(1)} &= A_f^{(0)}(I - \tilde{U}^{(0)}\tilde{L}^{(0)}) + A_s^{(0)}\tilde{L}^{(0)} \\ &= N + A_s^{(0)}\tilde{L}^{(0)} + \mathcal{O}(\varepsilon^2),\end{aligned}$$

where the term $A_s^{(0)}\tilde{L}^{(0)}$ can be written out explicitly by using the formulas (44a) and (44b) for the block components of Λ in the update formula (39):

$$A_s^{(0)}\tilde{L}^{(0)} = \Pi^\perp(\varepsilon[N, G])(\Lambda_{ff}^{(0)})^{-1},$$

where

$$\Pi^\perp := (Df^\top)^\perp ((N^\perp)^\top (Df^\top)^\perp)^{-1} (N^\perp)^\top.$$

A careful comparison to the matrix representation of oblique projection (Definition 2.5) reveals that in fact $\Pi^\perp = \Pi^S$ to leading order, when we evaluate this expression on the set $\mathcal{K}^{(0)}$. We also have $f = -\varepsilon(Df_0N_0)^{-1}(Df_0G_0) + \mathcal{O}(\varepsilon^2)$ and $(\Lambda_{ff}^{(0)})^{-1} = (Df_0N_0)^{-1} + \mathcal{O}(\varepsilon^2)$ on $\mathcal{K}^{(0)}$ (where we are using the 0-subscript convention in the previous lemma).

The CSP fiber $\mathcal{L}^{(1)}$ is defined on its corresponding CSP manifold $\mathcal{K}^{(1)}$ by Def. (33). Theorem 3 can be improved slightly such that the fiber approximation is still $\mathcal{O}(\varepsilon^j)$ -accurate if $A_f^{(j)}$ is evaluated on $\mathcal{K}^{(j-1)}$ (see Sec. 3.5 in [17]). The first-order corrections of the linear fast fibers and the CSP fibers are therefore equal. \square

Remark 6 *The formula in the preceding lemma simplifies to $k_1(x) = \Pi^S DGN(DfN)^{-1}$ when the linear fast fibers along the critical manifold are point-independent. This is convenient for chemical network applications admitting factorisations from stoichiometry. This also provides a new formula for the fast-fiber approximation in standard slow-fast systems.*

Remark 7 *Lemmas (46)–(46) should be considered in the context of previous work which interprets the CSP step in terms of curvature and higher-order geometric quantities [45]. For instance, the Lie bracket $[N, G]$ measures the extent to which the flows generated by the vector fields N_i and G fail to commute locally (for each $i = 1, \dots, n - k$) [29], and the first-order correction to the fast fibers records the projection of this bracket onto TS .*

5 Examples

We now demonstrate the two-step CSP method in several nonstandard examples. Our list of systems increases in complexity: first we consider a planar system where the slow manifold is equal to the critical manifold and the fast fiber bundle remains unchanged. Second, we consider a planar system where the slow manifold is equal to the critical manifold but the fast fiber bundle perturbs from the $\varepsilon = 0$ case. Third, we consider a planar system where both the manifold and fiber updates are nontrivial. Fourth, we revisit a three-dimensional system from the literature where the slow manifold is one-dimensional, and also contains a point where normal hyperbolicity is lost. Finally, we consider the four-dimensional system (3) discussed in the introduction.

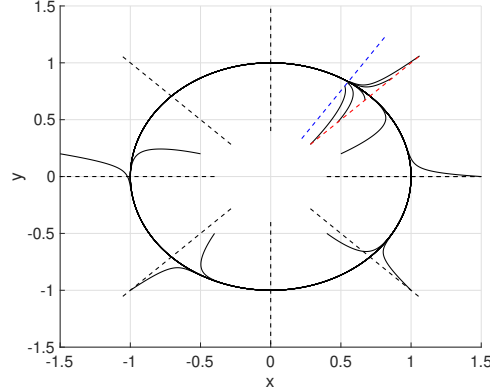


Figure 3: Several trajectories (black solid curves) plotted for system (48) (with $\varepsilon = 0.1$). Portions of the fast fibers given in (51) are given by dashed lines. The forward invariance of the family is also illustrated: trajectories on the red fiber $\mathcal{F}_\varepsilon(p(\pi/4))$ are flowed forward for a time $t = 2$. These trajectories all end on the blue fiber $\mathcal{F}_\varepsilon(p(\pi/4 + 2\varepsilon))$. Trajectories computed using a Dormand-Prince ODE solver in MATLAB R2018a [34].

5.1 Trivial updates of the slow manifold and fast fibers

Consider the following two-dimensional nonstandard system:

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} x \\ y \end{pmatrix} (1 - x^2 - y^2) + \varepsilon \begin{pmatrix} -y \\ x \end{pmatrix}. \quad (48)$$

The critical manifold $S = \{x^2 + y^2 = 1\}$ is a circle. The Jacobian evaluated along S is

$$DH|_S = \begin{pmatrix} -2x^2 & -2xy \\ -2xy & -2y^2 \end{pmatrix} \Big|_S, \quad (49)$$

with one trivial zero eigenvalue and one negative eigenvalue $\lambda = -2$ for all $(x, y) \in S$, implying that the critical manifold S is attracting and normally hyperbolic. Thus, Assumptions 2.1–2.3 are satisfied. Note that the origin is an isolated singularity of $N(z)$, where $f(z) \neq 0$, but we do not consider this singularity in the CSP iteration (see Remark 2).

When ε is small and positive, there is a clear separation between slow motion along S versus fast motion toward S . The dynamics is made obvious if we write the system in polar coordinates and plot a graph of representative trajectories (Fig. 3):

$$\begin{aligned} r' &= r(1 - r^2) \\ \theta' &= \varepsilon. \end{aligned} \quad (50)$$

The coordinate representation (50) decomposes the system into two independent ODEs. The invariant manifold $r = 1$, which is independent of ε , can be read off from the first equation of (50). Thus, $S_\varepsilon = S$. We can also determine that the (nonlinear) fast fiber bundle \mathcal{F}_ε is foliated by the family of rays extending from the origin, with basepoints on the circle:

$$\begin{aligned} \mathcal{F}_\varepsilon(p(\theta_0)) &= \{(r, \theta) : 0 < r < \infty, \theta = \theta_0\}, \quad p(\theta_0) = (1, \theta_0) \in S_\varepsilon \\ \mathcal{F}_\varepsilon &= \bigcup_{\theta_0 \in [0, 2\pi)} \mathcal{F}_\varepsilon(p(\theta_0)). \end{aligned} \quad (51)$$

Note that the nonlinear and linear fast fiber bundles coincide in this example: $\mathcal{F}_\varepsilon = \mathcal{N}_\varepsilon$. The fast fiber bundle is invariant as a family: for $t \in \mathbb{R}$, the fiber $\mathcal{F}_\varepsilon(p(\theta_0))$ is mapped to $\mathcal{F}_\varepsilon(p(\theta_0 + \varepsilon t))$ under the time t flow map. Furthermore, exponential contraction of the rays toward S_ε is governed by the equation $r' = r(1 - r^2)$. Compare these facts about the nonlinear fast fibers with Fenichel's theorem, Sec. 2.3. This behavior is similarly independent of the value of $\varepsilon > 0$.

We initialize the CSP two-step method using (40):

$$A^{(0)} = (N \quad (Df^\top)^\perp) = \begin{pmatrix} x & 2y \\ y & -2x \end{pmatrix} \quad (52a)$$

$$B^{(0)} = \frac{1}{2(x^2 + y^2)} \begin{pmatrix} 2x & 2y \\ y & -x \end{pmatrix}. \quad (52b)$$

We begin by computing the initial CSP manifold $\mathcal{K}^{(0)}$ (see (31)). We compute

$$\begin{aligned} B_{s^\perp}^{(0)} H &= \frac{1}{2(x^2 + y^2)} (2x \quad 2y) \left(\begin{pmatrix} x \\ y \end{pmatrix} (1 - x^2 - y^2) + \varepsilon \begin{pmatrix} -y \\ x \end{pmatrix} \right) \\ &= 1 - x^2 - y^2 = 0, \end{aligned} \quad (53)$$

and so

$$\mathcal{K}^{(0)} = \{(x, y) : x^2 + y^2 = 1\} = S.$$

We have

$$\begin{aligned} DA_f|_S &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ DA_s|_S &= \begin{pmatrix} 0 & 2 \\ -2 & 0 \end{pmatrix} \\ DH|_S &= \begin{pmatrix} -2x^2 & -2xy - \varepsilon \\ -2xy + \varepsilon & -2y^2 \end{pmatrix}. \end{aligned}$$

With this information, $\Lambda^{(0)}$ (defined in (30)) becomes

$$\Lambda^{(0)}|_S = \begin{pmatrix} -2 & 0 \\ 0 & 0 \end{pmatrix}. \quad (54)$$

Using (39), we find that $\tilde{U}^{(0)} = 0$ and $\tilde{L}^{(0)} = 0$.

The triviality of the updates implies that the CSP manifolds and fibers ((32)–(33)) are

$$\begin{aligned}\mathcal{K}^{(j)} &= \{(x, y) \in \mathbb{R}^2 : x^2 + y^2 = 1\} = S \\ \mathcal{L}^{(j)}(p) &= \{cp : c \in \mathbb{R}\}, \quad p \in S\end{aligned}$$

for $j = 0, 1, 2, \dots$.

5.2 Trivial updates of the slow manifold; nontrivial updates of the fast fibers

We now consider a variant of the previous system, where we modify the first component of $G(x, y)$:

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} x \\ y \end{pmatrix} (1 - x^2 - y^2) + \varepsilon \begin{pmatrix} -y + y^2(1 - x^2 - y^2) \\ x \end{pmatrix}. \quad (55)$$

We still have $S = \{(x, y) : x^2 + y^2 = 1\}$, and it is easy to check that this is also the invariant slow manifold for $\varepsilon > 0$: for $p = (x, y) \in S$ we have

$$\begin{aligned}H(x, y, \varepsilon) &= N(x, y, \varepsilon)f(x, y) + \varepsilon G(x, y, \varepsilon) \\ &= \varepsilon G(x, y, \varepsilon) \\ &= \begin{pmatrix} -\varepsilon y \\ \varepsilon x \end{pmatrix},\end{aligned}$$

so that $H(p, \varepsilon) \in T_p S$. Thus, $S = S_\varepsilon$ as before. In this modified system, however, the linear fast fiber $\mathcal{N}_{\varepsilon, p}$ will not be orthogonal to $T_p S_\varepsilon$ at points $p \in S_\varepsilon$.

The CSP step is initialized as usual with (40). The basis matrices are identical to (52a)–(52b) since we have not modified $N(z)$ or $f(z)$. From (30), the initial operator $\Lambda^{(0)}$ is (compare (54))

$$\Lambda^{(0)}|_S = \begin{pmatrix} -2 - 2\varepsilon xy^2 & 0 \\ \varepsilon y^3 & 0 \end{pmatrix}.$$

By definition (39), the update term $\tilde{U}^{(0)}$ is trivial since $\Lambda_{f_s}^{(0)} = 0$; on the other hand, the update quantity $\tilde{L}^{(0)}$ may give a nontrivial first-order correction to the fast fiber. The first column (resp. first row) of the updated basis matrix $A^{(1)}$ (resp. $B^{(1)}$) are

$$\begin{aligned}A_f^{(1)}|_S &= \begin{pmatrix} x + y^4 \varepsilon \\ y - xy^3 \varepsilon \end{pmatrix} + \mathcal{O}(\varepsilon^2) \\ B_{s\perp}^{(1)}|_S &= \begin{pmatrix} x & y \end{pmatrix}.\end{aligned}$$

Applying the definitions (32)–(33), the updated CSP objects are

$$\begin{aligned}\mathcal{K}^{(1)} &= \{B_{s\perp}^{(1)}H = 0\} \\ &= \{(x, y) \in \mathbb{R}^2 : x^2 + y^2 = 1\} \\ \mathcal{L}^{(1)}(x, y(x), \varepsilon) &= \left\{ c \left(\begin{pmatrix} x + y(x)^4\varepsilon \\ y - xy(x)^3\varepsilon \end{pmatrix} + \mathcal{O}(\varepsilon^2) \right) : c \in \mathbb{R} \right\}, \quad (x, y(x)) \in S.\end{aligned}$$

Here, the function $y(x)$ refers to a graph of $x^2 + y^2 = 1$ containing the chosen basepoint $(x, y(x))$. Graphs of the form $x(y)$ can also be used.

5.3 Parabolic critical manifold

Given the system

$$\begin{aligned}\begin{pmatrix} x' \\ y' \end{pmatrix} &= N(x, y)f(x, y) + \varepsilon G(x, y, \varepsilon) \\ &= \begin{pmatrix} -2x \\ -y \end{pmatrix} (x^2 + y - 1) + \varepsilon \begin{pmatrix} 2 \\ -x + \varepsilon \end{pmatrix}.\end{aligned}\tag{56}$$

The critical manifold is $S = \{f = 0\} = \{(x, y) \in \mathbb{R}^2 : y = 1 - x^2\}$. This critical manifold is globally attracting and normally hyperbolic—the Jacobian along S has one trivial zero eigenvalue and another eigenvalue $-(3x^2 + 1) < 0$. The attraction onto S_ε for $\varepsilon = 0.01$ is numerically demonstrated in Fig. 4.

The CSP method is initialized with the following basis and dual as given in (40):

$$\begin{aligned}A^{(0)} &= \begin{pmatrix} -2x & -1 \\ -y & 2x \end{pmatrix} \\ B^{(0)} &= \frac{1}{4x^2 + y} \begin{pmatrix} -2x & -1 \\ -y & 2x \end{pmatrix}.\end{aligned}$$

The initial CSP manifold (31) written to $\mathcal{O}(\varepsilon^0)$ order is

$$\mathcal{K}^{(0)} = \{(x, y) : y = 1 - x^2 + \mathcal{O}(\varepsilon)\}.$$

Define the auxiliary function $g(x) = 3x^2 + 1$. The operator $\Lambda^{(0)}$ (as defined in (30)) computed to linear order is

$$\Lambda^{(0)}|_{\mathcal{K}^{(0)}} = \begin{pmatrix} -g(x) - \frac{12x}{g(x)}\varepsilon & -3\frac{3x^2-1}{g(x)^2}\varepsilon \\ \frac{2(3x^2-2)}{g(x)}\varepsilon & -\frac{12x}{g(x)^2}\varepsilon \end{pmatrix} + \mathcal{O}(\varepsilon^2).$$

After one application of the two-step CSP method (37), we obtain the updated basis matrix

$$\begin{aligned}A^{(1)}|_{\mathcal{K}^{(0)}} &= \begin{pmatrix} A_f^{(1)} & A_s^{(1)} \end{pmatrix} \\ &= \begin{pmatrix} -2x + \frac{2(3x^2-2)}{g(x)^2}\varepsilon + & -1 + \frac{6x(3x^2-1)}{g(x)^3}\varepsilon \\ (x^2 - 1) - \frac{4(3x^3-2x)}{g(x)^2}\varepsilon & -2x - \frac{3(3x^4-4x^2+1)}{g(x)^3}\varepsilon \end{pmatrix} + \mathcal{O}(\varepsilon^2)\end{aligned}$$

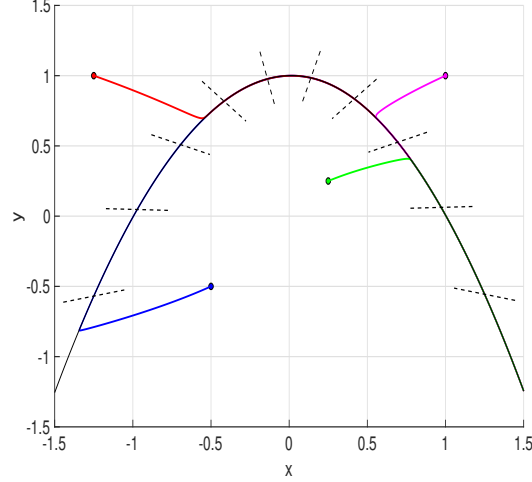


Figure 4: The attraction of four trajectories onto S_ε when $\varepsilon = 0.01$ in (56). Initial conditions for the blue, red, magenta, and green trajectories (denoted by dots) are $(-0.5, 0.5)$, $(-1.25, -1)$, $(1, 1)$, and $(0.25, 0.25)$, respectively. The parabolic critical manifold $S = \{y = 1 - x^2\}$ is given by the solid black line. Leading-order approximations of portions of the linear fast fibers (i.e. $N(z)$ for $z \in S$) are given by dashed line segments.

and dual $B^{(1)}|_{\mathcal{K}^{(0)}}$.

This gives us the first update of the CSP objects using the definitions (32)–(33):

$$\begin{aligned} \mathcal{K}^{(1)} &= \{(x, y) \in \mathbb{R}^2 : y = \psi^{(1)}(x) = 1 - x^2 + \frac{3x}{g(x)}\varepsilon + \mathcal{O}(\varepsilon^2)\} \\ \mathcal{L}^{(1)}(x, \psi^{(1)}(x)) &= \text{span Col}(A_f^{(1)}(x, \psi^{(1)}(x))) \\ &= \left\{ c \left(\begin{pmatrix} -2x + \frac{2(3x^2-2)}{g(x)^2}\varepsilon \\ (x^2-1) - \frac{4(3x^3-2x)}{g(x)^2}\varepsilon \end{pmatrix} + \mathcal{O}(\varepsilon^2) \right) : c \in \mathbb{R} \right\}. \end{aligned}$$

The $\Lambda^{(1)}$ update (30) is given by

$$\Lambda^{(1)}|_{\mathcal{K}^{(1)}} = \begin{pmatrix} -g(x) - \frac{12x}{g(x)}\varepsilon & 0 \\ 0 & -\frac{12x}{g(x)^2}\varepsilon \end{pmatrix} + \mathcal{O}(\varepsilon^2).$$

Observe that the off-diagonal elements now vanish (modulo nonzero $\mathcal{O}(\varepsilon^2)$ terms) while the diagonal terms remain stable up to order ε . As we continue to apply the CSP algorithm, the off-diagonal elements can be made to vanish modulo arbitrarily high orders; see Lemma 3. The order we used in the initial basis matrix implies that the (1,1) term governs the fast dynamics and (2,2)

term governs the slow dynamics in the decoupled system.

5.4 Three-species kinetics model

We consider the following reaction-kinetics toy model for three species x , y , and z :

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} -5x + 5y^2 - xy + z \\ 10x - 10y^2 - xy + z \\ +xy - z \end{pmatrix} + \varepsilon \begin{pmatrix} yz - x \\ -yz + x \\ -yz + x \end{pmatrix}. \quad (58)$$

This model is studied in [45], and an in-depth numerical analysis compares the CSP updates with various choices of initial conditions and two versions of the update rules. They give numerical evidence of nested three-timescale dynamics when $\varepsilon = 0.01$ by computing the spectrum of the Jacobian of the right-hand side of (58) along trajectories. Based on these calculations, they numerically approximate the (one-dimensional) trajectory in \mathbb{R}^3 corresponding to the decay of the two fastest modes. As noted in the paper, the eigenvectors are still relatively straightforward to evaluate symbolically in this problem, but this example is instructive in showing how we use the formalism to organise and simplify the calculations. Our first step is to observe that there is a factorisation which satisfies the assumptions of Section 2:

$$\begin{aligned} \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} &= N(x, y, z)f(x, y, z) + \varepsilon G(x, y, z) \\ &= \begin{pmatrix} -5 & -1 \\ 10 & -1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x - y^2 \\ xy - z \end{pmatrix} + \varepsilon \begin{pmatrix} yz - x \\ -yz + x \\ -yz + x \end{pmatrix}. \end{aligned}$$

Remark 8 *This factorisation is far from unique, but this does not affect the proceeding the argument. We remind the reader that such a factorisation can be obtained constructively, and furthermore the dimensions of the factors are constrained by the dimension of the critical manifold [9].*

The critical manifold is defined by $S = \{(x, y, z) : f(x, y, z) = 0\} \cap \{y \geq 0\}$:

$$S = \{(y^2, y, y^3) \in \mathbb{R}^3 : y \geq 0\}.$$

Assumptions 2.1 and 2.2 are therefore satisfied. We now turn to an analysis of the normal hyperbolicity of S . We have

$$DfN|_S = \begin{pmatrix} -5 - 20y & 1 + 2y \\ -5y + 10y^2 & y - y^2 - 1 \end{pmatrix},$$

from which

$$\begin{aligned}\operatorname{tr}(DfN|_S) &= -6 - 21y - y^2 < 0 \\ \det(DfN|_S) &= 5 + 20y + 45y^2 > 0.\end{aligned}$$

By Lemma 2, the critical manifold S is normally hyperbolic and attracting. Therefore, assumption 2.3 is also satisfied.

We now consider the reduced flow of the system. From (17), the projector onto the tangent space of S is given by

$$\begin{aligned}\Pi^S(y) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} -5 & -1 \\ 10 & -1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} -5 - 20y & 1 + 2y \\ -5y + 10y^2 & y - y^2 - 1 \end{pmatrix}^{-1} \begin{pmatrix} 1 & -2y & 0 \\ y & y^2 & -1 \end{pmatrix} \\ &= \frac{5}{g(y)} \begin{pmatrix} 4y & 2y & 6y \\ 2 & 1 & 3 \\ 6y^2 & 3y^2 & 9y^2 \end{pmatrix}.\end{aligned}$$

Observe that the image of Π^S is spanned at each point of S by the corresponding tangent vector to the curve $y \mapsto (y^2, y, y^3)$ parametrising S , as expected. In terms of this parametrization, the one-dimensional reduced flow along S (see Def. 2.4) is

$$\dot{y} = \frac{2y^2(1 - y^2)}{1 + 4y + 9y^2}.$$

The reduced flow vanishes at $y = 0$ and $y = 1$, corresponding to an unstable equilibrium $(0, 0, 0)$ and a stable equilibrium $(1, 1, 1)$ along S . Fenichel theory (Theorem 1) assures the existence of a one-dimensional, normally hyperbolic slow manifold S_ε near to S for $\varepsilon > 0$ sufficiently small, on which the invariant slow flow converges to the flow of the reduced system.

The analysis so far gives a theoretical underpinning to the dynamics shown in Fig. 5, as well as to the figures presented in Figs. 4 and 5 of [45], where a trajectory is tracked as it decays onto an apparent one-dimensional object which appears to lie close to the equilibria of the vector field. The existence of a spectral gap in compact neighborhoods of S_ε , for which numerical evidence is given in Fig. 3 of [45], is assured by the theory as $\varepsilon \rightarrow 0$. Furthermore, the direction of the flow once trajectories come near to the slow manifold can be deduced from the reduced flow analysis in the previous paragraph.

We now turn to the CSP method, computing analytically the first-order corrections to the slow manifold and the fast fibers. Using (40), the initial basis is given by

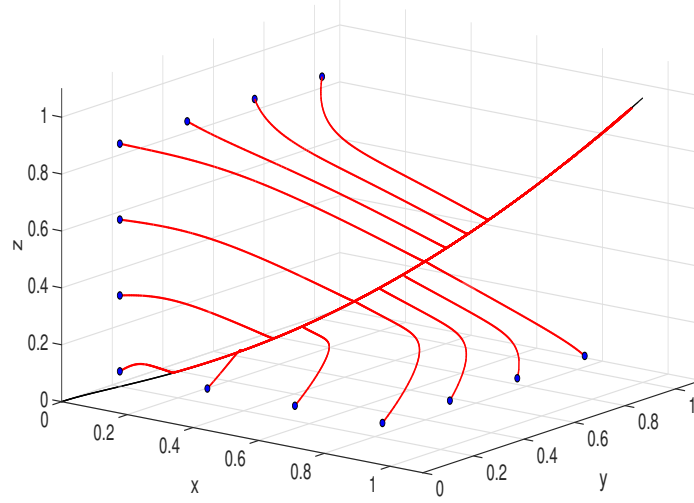


Figure 5: Numerical integration of several trajectories of (58) for $\varepsilon = 0.01$. The black curve is a portion of the critical manifold $S = \{(y^2, y, y^3) \in \mathbb{R}^3 : y \geq 0\}$.

$$A^{(0)} = \begin{pmatrix} -5 & -1 & \frac{2y}{x+2y^2} \\ 10 & -1 & \frac{1}{x+2y^2} \\ 0 & 1 & 1 \end{pmatrix}$$

and the dual by $B^{(0)} = (A^{(0)})^{-1}$. From the definition (31) and an application of Lemma 4, we can easily write down the first two CSP manifolds. We have

$$\begin{aligned} \mathcal{K}^{(0)} &= \{(x, y, z) : (x, z) = (y^2, y^3) + \mathcal{O}(\varepsilon)\}, \\ \mathcal{K}^{(1)} &= \{(x, y, z) : (x, z) = (y^2, y^3) + \varepsilon \frac{1}{g(y)} (p_1(y), p_2(y)) + \mathcal{O}(\varepsilon^2)\}, \end{aligned}$$

where

$$\begin{aligned} g(y) &= \det(DfN|_S) = 5 + 20y + 45y^2 \\ p_1(y) &= 6y^6 + 4y^5 - 6y^4 - 4y^3 \\ p_2(y) &= 6y^7 - 11y^6 - 26y^5 + 6y^4 + 20y^3 + 5y^2. \end{aligned}$$

We proceed to compute the analogous first-order approximations of the fibers using Lemma 5. Using Remark 6, we require only the projector Π^S and the Jacobian DG to derive the proper formula. We evaluate DG along S :

$$DG(y) = \begin{pmatrix} -1 & y^3 & y \\ 1 & -y^3 & -y \\ 1 & -y^3 & -y \end{pmatrix}.$$

This suffices to compute the first-order correction of the fast fiber immediately:

$$\begin{aligned} k_1(y) &= \Pi^S DGN(DfN)^{-1} \\ &= \frac{25}{g(y)^2} \begin{pmatrix} 12y^5 + 16y^4 + 8y^3 + 4y & -12y^4 + 16y^3 + 28y^2 \\ 6y^4 + 8y^3 + 4y^2 + 2 & -6y^3 + 8y^2 + 14y \\ 18y^6 + 24y^5 + 12y^4 + 6y^2 & -18y^5 + 24y^4 + 42y^3 \end{pmatrix}. \end{aligned}$$

The zeroth-order and first-order CSP fast fibers defined in (33) approximating the linear fast fibers of S_ε are therefore given by

$$\begin{aligned} \mathcal{L}^{(0)} &= \text{span Col}(A_f^{(0)}(y, \psi^0(y))) = \{Nc + \mathcal{O}(\varepsilon) : c \in \mathbb{R}^2\} \\ \mathcal{L}^{(1)} &= \text{span Col}(A_f^{(1)}(y, \psi^1(y))) = \{(N + \varepsilon k_1(y))c + \mathcal{O}(\varepsilon^2) : c \in \mathbb{R}^2\}. \end{aligned}$$

These and higher-order terms can be directly produced from the CSP iteration.

Remark 9 *An apparent nested three-timescale structure of the vector field (58) was noted in [45]. They provided numerical evidence of a second uniform gap in the spectrum, computed along a trajectory, and also observed the ‘intermediate’ relaxation of a sample trajectory along a (two-dimensional) surface before a final relaxation onto a (one-dimensional) curve. Consider the following two-parameter family of vector fields:*

$$\begin{aligned} \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} &= V_{\alpha, \varepsilon}(x, y, z) \\ &= \begin{pmatrix} -\alpha & -1 \\ 2\alpha & -1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x - y^2 \\ xy - z \end{pmatrix} + \varepsilon \begin{pmatrix} yz - x \\ -yz + x \\ -yz + x \end{pmatrix} \\ &= \alpha \begin{pmatrix} -1 \\ 2 \\ 0 \end{pmatrix} (x - y^2) + \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix} (xy - z) + \varepsilon \begin{pmatrix} yz - x \\ -yz + x \\ -yz + x \end{pmatrix} \\ &= \alpha N_1 f_1 + N_2 f_2 + \varepsilon G. \end{aligned}$$

The system (58) was studied for the parameter set $(\alpha, \varepsilon) = (5, 0.01)$ in [45], whereas our analysis fixes only $\alpha = 5$ so that we can apply Fenichel theory to the one-parameter family $V_{5, \varepsilon}$ of singularly perturbed systems as $\varepsilon \rightarrow 0$. In this context, there are only two distinguished timescales of the system.

From the point of view of geometric singular perturbation theory, recovering a three-timescale structure of slow manifolds requires that we consider the full two-parameter family $V_{\alpha,\varepsilon}$ in the regime $\alpha \gg 1$ and $\varepsilon \ll 1$. For $\alpha > 0$, we rescale time by $s = \alpha t$ and let $\delta = 1/\alpha$. Then (letting primes denote differentiation by s) we have

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = N_1 f_1 + \delta(N_2 f_2 + \varepsilon G). \quad (59)$$

The system is now in a factored form which has recently been studied in non-standard multiple-timescale systems having a nested three-timescale structure: a hierarchy of timescales is reflected in a nesting of invariant, normally hyperbolic submanifolds in the singular limit $\varepsilon, \delta \rightarrow 0$ [2, 24]. In particular, for systems of the form (59), nested versions of the projector Π^S can also be computed. We proceed no further with a rigorous analysis of the three-timescale structure, but point out that adapting our results for nonstandard CSP algorithms to the m -timescale case (with $m \geq 2$) is likely to be a fruitful avenue for further work. The splitting in (59) should also be compared to the three-term splitting written down in [45].

5.5 Stiefenhofer's slime cell model

Recall system (3):

$$\begin{pmatrix} p' \\ d' \\ r' \\ b' \end{pmatrix} = \begin{pmatrix} 2 & 2 \\ 0 & 1 \\ 1 & 0 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} -k_5 r p^2 + k_{-5} b \\ -k_4 d p^2 + k_{-4}(c - d - r - b) \end{pmatrix} + \varepsilon \begin{pmatrix} k_3 - k_{-3} p + k_2 S b \\ -k_1 d + k_{-1} r \\ k_1 d - k_{-1} r \\ 0 \end{pmatrix} \quad (60)$$

for parameters $k_i, S, c > 0$, together with the perturbation parameter $\varepsilon > 0$. This system has the factorized form $H(z) = N(z)f(z) + \varepsilon G(z, \varepsilon)$. Using (40), the initial basis is given by

$$A^{(0)} = \begin{pmatrix} 2 & 2 & \frac{k_{-5}}{2k_5 p r} & -\frac{p}{2r} \\ 0 & 1 & -\frac{k_4 k_{-5} d + k_{-4} k_5 r}{k_5(k_4 p^2 + k_{-4})r} & -\frac{k_{-4} r - k_4 d p^2}{(k_4 p^2 + k_{-4})r} \\ 1 & 0 & 0 & 1 \\ -1 & 0 & 1 & 0 \end{pmatrix}$$

and the dual by $B^{(0)} = (A^{(0)})^{-1}$, whose first two rows are given by the 2×4 matrix $(DfN)^{-1}Df$.

As before, the leading-order term of the graph of $\mathcal{K}^{(0)}$ (defined in (31)) will match the graph of $\{f = 0\}$:

$$\mathcal{K}^{(0)} = \left\{ (p, d, r, b) : (r, b) = \psi^{(0)}(p, d) = (k_{-5}\alpha(p, d), k_5 p^2 \alpha(p, d)) + \mathcal{O}(\varepsilon) \right\},$$

where

$$\alpha(p, d) = \frac{-k_4 dp^2 + k_{-4}(c-d)}{k_{-4}(k_5 p^2 + k_{-5})}.$$

Applying the CSP manifold definition (32), we have

$$\mathcal{K}^{(1)} = \{(p, d, r, b) : (r, b) = \psi_0^{(1)}(p, d) + \varepsilon \psi_1^{(1)}(p, d) + \mathcal{O}(\varepsilon^2)\},$$

where $\psi_0^{(1)}(p, d) = \psi_0^{(0)}(p, d)$ and the first-order correction $\psi_1^{(1)}(p, d)$ can be factored as

$$\psi_1^{(1)}(p, d) = \frac{1}{\gamma(p)}(\beta_2(p)d^2 + \beta_1(p)d + \beta_0(p), \delta_2(p)d^2 + \delta_1(p)d + \delta_0(p)),$$

for the seven polynomials $\beta_i, \delta_i, \gamma$ in p , defined as follows:

$$\begin{aligned} \gamma(p) = & (k_{-4}^2(k_{-5} + k_5 p^2)^2(-4dk_4^2 k_5 k_{-5} p^5 + k_{-4}^2(k_{-5}^2 + k_5^2 p^4 + 2k_5 k_{-5} p(2c - 2d + p)) + \\ & k_4 k_{-4} p(4d(k_{-5}^2 + k_5^2 p^4) + p(k_{-5}^2 + k_5^2 p^4 + 2k_5 k_{-5} p(2c + p)))) \end{aligned}$$

$$\begin{aligned} \beta_2(p) = & k_2 k_4 k_{-1} k_1 p(-2k_2 k_4 k_5^3 k_{-4} k_{-5}(k_4 p^2 + k_{-4})Sp^6 - 4k_4 k_5^2 k_{-1} k_{-4} k_{-5}^2(k_4 p^2 + k_{-4})p^4 + \\ & 4k_4 k_5^2 k_{-1} k_{-4}^2 k_{-5}(k_4 p^2 + k_{-4})p^4 + 4k_4^2 k_5 k_5 k_{-5}^2(k_{-5} - k_{-4})(k_4 p^2 + k_{-4})p^4 + \\ & 4k_1 k_4 k_5 k_{-4}(k_{-4} - k_{-5})(k_5 k_{-4} - k_4 k_{-5})(k_5 p^2 + k_{-5})p^4 - 2k_2 k_4 k_5 k_{-4} k_{-5}^3(k_4 p^2 + k_{-4})Sp^2 + \\ & 2k_3 k_5^2 k_{-4} k_{-5}(k_4 p^2 + k_{-5})(k_4^2 p^4 + 2k_{-4}(k_{-4} - k_{-5})p^2 + k_{-4}^2)Sp^2) \end{aligned}$$

$$\begin{aligned} \beta_1(p) = & p(-2k_4 k_5^3 k_{-3} k_{-4}^2 k_{-5} p^7 + 2ck_2 k_4 k_5^3 k_{-4}^2 k_{-5} Sp^6 - k_4 k_5^2 k_{-1} k_{-4} k_{-5}^2(k_4 p^2 + k_{-4})p^5 + \\ & k_4 k_5^2 k_{-1} k_{-4}^2 k_{-5}(k_4 p^2 + k_{-4})p^5 + k_1 k_4 k_5^2 k_{-4}^2(k_{-4} - k_{-5})(k_5 p^2 + k_{-5})p^5 + \\ & 4ck_4 k_5^2(k_1 - k_{-1})k_{-4}^2(k_{-4} - k_{-5})k_{-5} p^4 - 8ck_4^2 k_5 k_{-1} k_{-4} k_{-5}^2(k_{-5} - k_{-4})p^4 + \\ & k_4 k_5 k_{-1} k_{-4}(k_{-4} - 2k_{-5})k_{-5}^2(k_4 p^2 + k_{-4})p^3 + k_5^2 k_{-1} k_{-4}^3 k_{-5}(k_4 p^2 + k_{-4})p^3 + \\ & k_1 k_5 k_{-4}^2(k_5 k_{-4}^2 + k_4(k_{-4} - 2k_{-5})k_{-5})(k_5 p^2 + k_{-5})p^3 + 2k_5^2 k_{-3} k_{-4}^2 k_{-5}(k_4^2 p^4 + k_4(2k_{-4} - 3k_{-5})p^2 + \\ & k_{-4}^2)p^3 - 4ck_4 k_5 k_{-1} k_{-4}^2 k_{-5}^2(k_{-5} - k_{-4})p^2 - 4ck_2 k_5^2 k_{-4}^2 k_{-5}(k_4^2 p^4 + k_4(2k_{-4} - k_{-5})p^2 + \\ & k_{-4}^2)Sp^2 + 2ck_4 k_5 k_{-4}^2 k_{-5}^2(2k_1 k_{-4} - 2k_1 k_{-5} + k_2 k_{-5} S)p^2 + \\ & k_5 k_{-1} k_{-4}^3 k_{-5}^2(k_4 p^2 + k_{-4})p - k_1 k_4 k_{-4}^2 k_{-5}^3(k_5 p^2 + k_{-5})p + \\ & k_1 k_5 k_{-4}^4 k_{-5}(k_5 p^2 + k_{-5})p + 2k_5 k_{-3} k_{-4}^2 k_{-5}^2(k_4^2 p^4 + k_4(2k_{-4} - 3k_{-5})p^2 + \\ & k_{-4}^2)p - k_4 k_{-4} k_{-5}^4(2k_{-3} k_{-4} + k_{-1}(k_4 p^2 + k_{-4}))p + 2k_3 k_{-4}^2 k_{-5}(k_5 p^2 + k_{-5})(k_4 k_5(k_5 - k_4)p^4 + \\ & 2k_4 k_5(k_{-5} - k_{-4})p^2 - k_5 k_{-4}^2 + k_4 k_{-5}^2)) \end{aligned}$$

$$\begin{aligned} \beta_0(p) = & p(ck_4 k_5^2 k_{-4}^2 k_{-5}((-k_{-1} - 2k_{-3})k_{-4} + k_{-1} k_{-5})p^5 - ck_4 k_5 k_{-1} k_{-4}^2(k_{-4} - 2k_{-5})k_{-5}^2 p^3 + \\ & ck_5^2(-k_{-1} - 2k_{-3})k_{-4}^4 k_{-5} p^3 + 2c^2 k_5 k_{-4}^2 k_{-5}(2k_4 k_{-1} k_{-5}(k_{-5} - k_{-4}) + \\ & k_2 k_5 k_{-4}(k_4 p^2 + k_{-4})S)p^2 + ck_4 k_{-1} k_{-4}^2 k_{-5} p - ck_5 k_{-1} k_{-4}^4 k_{-5}^2 p - 2ck_5 k_{-3} k_{-4}^3 k_{-5}^2(k_4 p^2 + k_{-4})p + \\ & 2ck_3 k_5 k_{-4}^3 k_{-5}(k_4 p^2 + k_{-4})(k_5 p^2 + k_{-5})) \end{aligned}$$

$$\begin{aligned} \delta_2(p) = & -k_5 p(-4k_4^2 k_5 k_{-1} k_{-5}^2 (k_4 p^2 + k_{-4}) p^6 + 4k_4 k_5^2 k_{-1} k_{-4} k_{-5} (k_4 p^2 + k_{-4}) p^6 + 4k_1 k_4 k_5^2 k_{-4}^2 (k_5 p^2 + k_{-5}) p^6 \\ & - 4k_1 k_4^2 k_5 k_{-4} k_{-5} (k_5 p^2 + k_{-5}) p^6 - 4k_4^2 k_{-1} k_{-4} k_{-5}^2 (k_4 p^2 + k_{-4}) p^4 + \\ & 4k_4 k_5 k_{-1} k_{-4}^2 k_{-5} (k_4 p^2 + k_{-4}) p^4 + 4k_1 k_4 k_5 k_{-4}^3 (k_5 p^2 + k_{-5}) p^4 - 4k_1 k_4^2 k_{-4}^2 k_{-5} (k_5 p^2 + k_{-5}) p^4 + \\ & 2k_2 k_5 k_{-4} (k_4 p^2 + k_{-4}) (k_4 k_5^2 p^6 + k_4 (k_4 + 2k_5) k_{-5} p^4 + k_4 k_{-5} (2k_{-4} + k_{-5}) p^2 + k_{-4}^2 k_{-5} S p^2) \end{aligned}$$

$$\begin{aligned} \delta_1(p) = & -k_5 p(k_4 k_5^2 k_{-1} k_{-4} k_{-5} (k_4 p^2 + k_{-4}) p^7 + k_1 k_4 k_5^2 k_{-4}^2 (k_5 p^2 + k_{-5}) p^7 + \\ & 8ck_4^2 k_5 k_{-1} k_{-4} k_{-5}^2 p^6 - 4ck_4 k_5^2 k_{-1} k_{-4}^2 k_{-5} p^6 + 2k_4 k_5 k_{-1} k_{-4} k_{-5}^2 (k_4 p^2 + k_{-4}) p^5 + \\ & k_4 k_5 k_{-1} k_{-4}^2 k_{-5} (k_4 p^2 + k_{-4}) p^5 + k_1 k_4 k_5 k_{-4}^3 (k_5 p^2 + k_{-5}) p^5 + \\ & 2k_1 k_4 k_5 k_{-4}^2 k_{-5} (k_5 p^2 + k_{-5}) p^5 + 4ck_4 (2k_4 + k_5) k_{-1} k_{-4}^2 k_{-5}^2 p^4 - \\ & 4ck_4 k_5 k_{-1} k_{-4}^3 k_{-5} p^4 + k_4 k_{-1} k_{-4} k_{-5}^3 (k_4 p^2 + k_{-4}) p^3 + \\ & k_4 k_{-1} k_{-4}^2 k_{-5}^2 (k_4 p^2 + k_{-4}) p^3 + k_1 k_4 k_{-4}^2 k_{-5}^2 (k_5 p^2 + k_{-5}) p^3 + \\ & k_1 k_4 k_{-4}^3 k_{-5} (k_5 p^2 + k_{-5}) p^3 + 4ck_4 k_{-1} k_{-4}^3 k_{-5}^2 p^2 + 4ck_1 k_4 k_{-4}^2 k_{-5} (k_5 p^2 + k_{-4}) (k_5 p^2 + k_{-5}) p^2 - \\ & 2ck_2 k_5 k_{-4}^2 (k_4 k_5^2 p^6 + 2k_4 (k_4 + k_5) k_{-5} p^4 + k_4 k_{-5} (4k_{-4} + k_{-5}) p^2 + 2k_{-4}^2 k_{-5} S p^2 + \\ & k_1 k_{-4}^4 (k_5 p^2 + k_{-5})^2 p + k_{-1} k_{-4}^3 k_{-5} (k_4 p^2 + k_{-4}) (k_5 p^2 + k_{-5}) p + \\ & 2k_{-3} k_{-4}^2 (k_5 p^2 + k_{-5}) (k_4 k_5^2 p^6 + k_4 (k_4 + 2k_5) k_{-5} p^4 + k_4 k_{-5} (2k_{-4} + k_{-5}) p^2 + k_{-4}^2 k_{-5} p - \\ & 2k_3 k_{-4}^2 (k_5 p^2 + k_{-5}) (k_4 k_5^2 p^6 + k_4 (k_4 + 2k_5) k_{-5} p^4 + k_4 k_{-5} (2k_{-4} + k_{-5}) p^2 + k_{-4}^2 k_{-5})) \end{aligned}$$

$$\begin{aligned} \delta_0(p) = & -k_5 p(-ck_4 k_5^2 k_{-1} k_{-4}^2 k_{-5} p^7 - 2ck_4 k_5 k_{-1} k_{-4}^2 k_{-5}^2 p^5 - \\ & ck_4 k_5 k_{-1} k_{-4}^3 k_{-5} p^5 - ck_4 k_{-1} k_{-4}^2 k_{-5}^3 p^3 - ck_4 k_{-1} k_{-4}^3 k_{-5}^2 p^3 + \\ & 2c^2 k_{-4}^2 k_{-5} (k_2 k_5 k_{-4} (k_4 p^2 + k_{-4}) S - 2k_4 k_{-1} k_{-5} (k_5 p^2 + k_{-4})) p^2 - \\ & ck_{-1} k_{-4}^4 k_{-5} (k_5 p^2 + k_{-5}) p - 2ck_{-3} k_{-4}^3 k_{-5} (k_4 p^2 + k_{-4}) (k_5 p^2 + k_{-5}) p + \\ & 2ck_3 k_{-4}^3 k_{-5} (k_4 p^2 + k_{-4}) (k_5 p^2 + k_{-5})). \end{aligned}$$

The fast fiber update, which we do not write down, will be an $\mathcal{O}(\varepsilon)$ correction to the first 4×2 block of $A^{(0)}$, in analogy to the previous examples.

Remark 10 *The tensorial nature of the update step only becomes apparent in systems with dimension higher than two. For example, to compute $\Lambda_{fs}^{(0)}$, we must compute the tensor $DA_s^{(0)}$. Such computations quickly become unwieldy for high-dimensional systems after the first or second CSP iterate.*

Remark 11 *Trajectories in the Figs. 1,3,4, and 5 were computed using a Dormand-Prince ODE solver in MATLAB R2018a [34]. Symbolic computations for these examples were performed using Mathematica Version 11.1.1.0 [48]. An example notebook file demonstrating these calculations for (60) has been uploaded to <https://github.com/ianlizarraga/Nonstandard-CSP->.*

6 Conclusion

We have given a detailed treatment of the CSP method for nonstandard slow-fast systems (7), when the vector field admits a geometrically intuitive factorization in the leading-order term, and demonstrated the method explicitly for nontrivial examples. There appear to be several other natural connections between the CSP algorithm and this factorization, which we comment on further.

6.1 CSP as projection

There is a tantalizing connection between the CSP two-step update and the projection operators (12)–(13) which were naturally induced by the normally hyperbolic splitting. In the examples 5.1 and 5.2, Π^S is an orthogonal projection onto $T_z S$, and furthermore the manifold $S = S_\varepsilon$ is given by $f = 0$ exactly. Per Lemma 5, the computation (48) shows that the fast fiber update is trivial if $[N, G] \in \ker \Pi^S$. This is indeed the case in the first example 5.1 but not in the modification 5.2.

In view of Remark 7, it is clearly worthwhile to probe deeper geometric connections between the CSP update step and the projectors which define the fast and slow subsystems of (7). One step in this direction is a complete geometric recasting of the iteration as a method which updates the projectors themselves, initialising with the projectors naturally induced by the factorisation $h_0(z) = N(z)f(z)$.

6.2 CSP as a factorization algorithm for nonstandard vector fields

As discussed in Sec. 2, the leading-order factorization gives a compact description of the geometry of the system near the critical manifold S when $\varepsilon = 0$, and gives approximate information about the dynamics on the nearby slow manifold S_ε when $\varepsilon > 0$. Consider the following conjecture.

Conjecture 1 *Given system (7) under the Assumptions 2.1–2.3, there exists a corresponding factorisation*

$$H(z, \varepsilon) = N_\varepsilon(z, \varepsilon)f_\varepsilon(z, \varepsilon) + \varepsilon\tilde{G}(z, \varepsilon),$$

where the new objects $N_\varepsilon(z, \varepsilon)$, $f_\varepsilon(z, \varepsilon)$, and $\tilde{G}(z, \varepsilon)$ satisfy the following properties:

- (Slow manifold as a level set) $S_\varepsilon = \{z \in \mathbb{R}^n : f_\varepsilon(z, \varepsilon) = 0\}$.
- (Basis of fast fibers) The columns of $N_\varepsilon(p, \varepsilon)$ span the linear fast fibers $\mathcal{N}_\varepsilon(p)$ at basepoints $p \in S_\varepsilon$.
- (Invariance) $\tilde{G}(p, \varepsilon) \in T_p S_\varepsilon$ for $p \in S_\varepsilon$.

The assertion is that a vector field factorization with respect to the critical manifold S when $\varepsilon = 0$ will induce a new factorization with respect to the slow manifold S_ε when $\varepsilon > 0$.

We describe a possible direction to answer this conjecture in the affirmative in the special case where $S_\varepsilon = S$ (as in the examples 5.1 and 5.2). The idea is to use the CSP method to obtain iterative refinements of the objects $N_\varepsilon(z, \varepsilon)$, $f_\varepsilon(z, \varepsilon)$, and $\tilde{G}(z, \varepsilon)$. Writing out the first few terms in the asymptotic series of the CSP fast fiber $\mathcal{L}^{(1)}$ (see (33) and (37)), we have $A_f^{(1)}(z, \varepsilon) = N(z) + \varepsilon A_{f,1}^{(1)}(z) + \mathcal{O}(\varepsilon^2)$.

The vector field can be re-factorized as follows:

$$\begin{aligned} H(z, \varepsilon) &= N(z)f(z) + \varepsilon G(z, \varepsilon) \\ &= N(z)f(z) + \varepsilon A_{f,1}^{(1)}(z)f(z) - \varepsilon A_{f,1}^{(1)}(z)f(z) + \varepsilon G(z, \varepsilon) \\ &= (N(z) + \varepsilon A_{f,1}^{(1)}(z))f(z) + \varepsilon G^{(1)}(z, \varepsilon), \\ &= N^{(1)}(z, \varepsilon)f^{(1)}(z) + \varepsilon G^{(1)}(z, \varepsilon), \end{aligned}$$

where

$$\begin{aligned} f^{(1)}(z) &:= f(z) \\ N^{(1)}(z, \varepsilon) &:= N(z) + \varepsilon A_{f,1}^{(1)}(z) \\ G^{(1)}(z, \varepsilon) &:= G(z, \varepsilon) - A_{f,1}^{(1)}(z)f(z). \end{aligned}$$

In comparison to the original factorization $H = Nf + \varepsilon G$, this new factorization has ε -dependence in the ‘leading-order’ term $N^{(1)}f^{(1)}$, and a modified ‘remainder’ term $G^{(1)}$. But observe that $S = S_\varepsilon = \{f^{(1)} = 0\}$. Furthermore, the column space of the prefactor matrix $N^{(1)}$ is now an $\mathcal{O}(\varepsilon)$ -approximation of the fast fibers. Finally, $G^{(1)}(z, \varepsilon)|_S = G(z, \varepsilon) \in T_p S$ since S is invariant by assumption.

We can extend this idea in the obvious way to refine the factorization to some arbitrary order j :

$$\begin{aligned} H(z, \varepsilon) &= N^{(j)}(z, \varepsilon)f^{(j)}(z) + \varepsilon G^{(j)}(z, \varepsilon), \\ f^{(j)}(z) &:= f(z) \\ N^{(j)}(z, \varepsilon) &:= N(z) + \sum_{i=1}^j \varepsilon^i A_{f,i}^{(j)}(z) \\ G^{(j)}(z, \varepsilon) &:= G(z, \varepsilon) - \sum_{i=1}^j \varepsilon^{i-1} A_{f,i}^{(j)}(z)f(z). \end{aligned}$$

We remind the reader that the triviality of the level set update $f^{(j)} = f$ is a consequence of the assumption that $S = S_\varepsilon$. The general case where the CSP

manifolds also update nontrivially is a topic of further study. Here, more care must be taken to write down the factorizations since the fiber basepoints are not fixed. Furthermore, nontrivial cross-terms of the form $N^{(k)}f^{(l)}$, where $k+l > j$, begin to appear at a given iterate j .

6.3 CSP for slow manifolds of saddle-type

Normally hyperbolic slow manifolds of saddle-type arise in traveling-wave profiles of the FitzHugh-Nagumo model [3], in the Hodgkin-Huxley model [12], and in models of cardiac pacemakers [23]. Saddle-type slow manifolds and their fast fibers are challenging to numerically approximate even in the standard case, due to exponential instabilities in both forward and backward time [1, 6, 11, 22, 46]. It is therefore of interest to relax the assumption that the critical manifold be attracting for the CSP method.

References

- [1] H.W. BROER, H.M. OSINGA, AND G. VEGTER, *Computing a normally hyperbolic invariant manifold of saddle type*, in G.S. Ladde and M. Sambandham (Eds.), *Proceedings of Dynamic Systems and Applications 2(1996)*, pp. 83–90
- [2] P.T. CARDIN AND M.A. TEIXEIRA, *Fenichel Theory for Multiple Time Scale Singular Perturbation Problems*, *SIAM J. Appl. Dyn. Syst.*, 6 (2017), pp. 1425-1452.
- [3] A. R. CHAMPNEYS, V. KIRK, E. KNOBLOCH, B. E. OLDEMAN, AND J. SNEYD, *When Shil'nikov meets Hopf in excitable system*, *SIAM J. Appl. Dyn. Syst.*, 6 (2007), pp. 663-693.
- [4] M.J. DAVIS AND R.T. SKODJE, *Geometric investigation of low-dimensional manifolds in systems approaching equilibrium*, *J. Chem. Phys.*, 111(1999), pp. 859–874.
- [5] H. DEGN, L.F. OLSEN, AND J.W. PERRAM, *Bistability, oscillation, and chaos in an enzyme reaction*, *Annals New York Acad. Sci.*, 316(1979), pp. 623-627.
- [6] S. FARJAMI, V. KIRK, AND H.M. OSINGA, *Computing the Stable Manifold of a Saddle Slow Manifold*, *SIAM J. Appl. Dyn. Syst.*, 17 (2018), pp. 350–379.
- [7] N. FENICHEL, *Geometric singular perturbation theory for ordinary differential equations*, *J. Differential Equations*, 31(1979), pp. 53–98.

- [8] C.W. GEAR AND I.G. KEVREKIDIS, *Constraint-Defined Manifolds: a Legacy Code Approach to Low-Dimensional Computation*, J. Sci. Comp., 25(2005), 17–28.
- [9] A. GOEKE AND S. WALCHER, *Quasi-Steady State: Searching for and Utilizing Small Parameters*, Springer Proceedings in Mathematics and Statistics, 35(2013), 153–178.
- [10] A. GOEKE AND S. WALCHER, *A constructive approach to quasi-steady state reduction*, J. Math. Chem., 52(2014), pp. 2596–2626.
- [11] J. GUCKENHEIMER AND C. KUEHN, *Computing Slow Manifolds of Saddle Type*, SIAM J. Appl. Dyn. Syst., 8 (2009), pp. 854–879.
- [12] C.R. HASAN, B. KRAUSKOPF, AND H.M. OSINGA, *Saddle Slow Manifolds and Canard Orbits in R^4 and Application to the Full Hodgkin-Huxley Model*, J. Math. Neurosci. (2018) 8:5.
- [13] N. HINRICHS, M. OESTREICH, K. POPP, *On the modelling of friction oscillators*, Journal of Sound and Vibration, 216(1998), pp. 435–459.
- [14] C.K.R.T. JONES, *Geometric singular perturbation theory*, Lect. Notes. Math, 1609(1995), pp. 44–118.
- [15] B.O. PALSSON AND E. N. LIGHTFOOT, *Mathematical modelling of dynamics and control in metabolic networks. I. On Michaelis-Menten kinetics*, J. Theoret. Biol., 111(1984), pp. 273–302.
- [16] A. ZAGARIS, H.G. KAPER, AND T.J. KAPER, *Analysis of the Computational Singular Perturbation Reduction Method for Chemical Kinetics*, J. Nonlinsci. 14(2004), pp. 59–91.
- [17] A. ZAGARIS, H.G. KAPER, AND T.J. KAPER, *Fast and Slow Dynamics for the Computational Singular Perturbation Method*, Multiscale Model. Simul., 2(2004), pp. 613–638.
- [18] A. ZAGARIS, H.G. KAPER, AND T.J. KAPER, *Two perspectives of reduction of ordinary differential equations*, Math. Nachr., 278(2005), pp. 1629–1642.
- [19] H.G. KAPER, T.J. KAPER, AND A. ZAGARIS, *Geometry of the Computational Singular Perturbation Method*, Math. Model. Nat. Phenom., 10(2015), pp. 16–30.
- [20] J. KEENER AND J. SNEYD, *Mathematical Physiology*, Interdisciplinary Applied Mathematics: Mathematical Biology, 8, Springer, Hong Kong, 1998.
- [21] E.F. KELLER AND L.A. SEGEL, *Model for chemotaxis*, J. Theoret. Biol., 30(1971), pp. 225–234.

- [22] K. ULDALL KRISTIANSEN, *Computation of Saddle-Type Slow Manifolds Using Iterative Methods*, SIAM J. Appl. Dyn. Syst., 14(2), 1189–1227.
- [23] T. KROGH-MADSEN, L. GLASS, E. DOEDEL, AND M. GUEVARA, *Apparent discontinuities in the phasetting response of cardiac pacemakers*, J. Theoret. Biol., 230 (2004), pp. 499–519.
- [24] N. KRUFF AND S. WALCHER, *Coordinate-independent singular perturbation reduction for systems with three time scales*, Math Biosci Eng. 16(5):5062–5091.
- [25] C. KUEHN, *Multiple Time Scale Dynamics*, Springer International Publishing Switzerland, 2015.
- [26] C. KUEHN AND P. SZMOLYAN, *Multiscale Geometry of the Olsen Model*, J. Nonlinear Sci., 25(2015), 583–629.
- [27] S.H. LAM AND D.A. GOUSSIS, *Understanding complex chemical kinetics with computational singular perturbation*, Symposium (International) on Combustion, 22(1989), pp. 931–941.
- [28] S.H. LAM AND D.A. GOUSSIS, *The CSP Method for Simplifying Kinetics*, Int. J. Chem. Kinetics, 26(1994), pp. 461–486.
- [29] S. LANG, *Differential and Riemannian Manifolds*, Graduate Texts in Mathematics, vol. 160, 3rd edn. Springer, New York (1995).
- [30] T. LU AND C.K. LAW, *Strategies for mechanism reduction for large hydrocarbons: n-heptane*, Combustion and Flame, 154(2008), pp. 153–163.
- [31] U. MAAS AND S.B. POPE, *Implementation of simplified chemical kinetics based on intrinsic low-dimensional manifolds*, Proceedings of the 24th International Symposium on Combustion (1992), pp. 103–112.
- [32] U. MAAS AND S.B. POPE, *Simplifying Chemical Kinetics: Intrinsic Low-Dimensional Manifolds in Composition Space*, Combustion and Flame, 88(1992), pp. 239–264.
- [33] A. MASSIAS, D. DIAMANTIS, E. MASTORAKOS, AND D. GOUSSIS, *An algorithm for the construction of global reduced mechanisms with CSP data*, Combustion and Flame, 117(1999), pp. 685–708.
- [34] THE MATHWORKS, INC., *MATLAB, Version 9.4.0 (R2018a)*, Natick, Massachusetts (2018).
- [35] K.D. MEASE, *Geometry of Computational Singular Perturbations*, IFAC Proceedings Volumes, 28(1995), pp. 855–861.
- [36] L. NOETHEN AND S. WALCHER, *Tikhonov’s theorem and quasi-steady state*, Discrete and Continuous Dynamical Systems - Series B 16(3) (2011), 945–961.

- [37] A.V. RAO AND K.D. MEASE, *Dichotomic basis approach to solving hypersensitive optimal control problems*, *Automatica* 35(1999), pp. 633–642.
- [38] A.J. ROBERTS, *Computer algebra derives correct initial conditions for low-dimensional dynamical models*, *Comput. Phys. Commun.* 126(2000), pp. 187–206.
- [39] A.J. ROBERTS, *Normal form transforms separate slow and fast modes in stochastic dynamical systems*, *Physica A*, 387(2008), pp. 12–38.
- [40] M. SCHAUER AND R. HEINRICH, *Quasi-Steady-State Approximation in the Mathematical Modelling of Biochemical Reaction Networks*, *Math. Biosci.*, 65(1983), 155–171.
- [41] M. STIEFENHOFER, *Quasi-steady-state approximation for chemical reaction networks*, *J. Math. Biol.*, 36(1998), 593–609.
- [42] A. N. TIKHONOV, *Systems of differential equations containing small parameters in the derivatives*, *Mat. Sb. N.S.* 31(73) (1952), 575–586.
- [43] M. VALORANI AND D. GOUSSIS, *Explicit time-scale splitting algorithm for stiff problems: auto-ignition of gaseous-mixtures behind a steady shock*, *J. Comput. Phys.* 168(2001), 1–36.
- [44] M. VALORANI, H. NAJM, AND D. GOUSSIS, *CSP analysis of a transient flame vortex interaction: time scales and manifolds*, *Combustion and Flame* 134(2003), 35–53.
- [45] M. VALORANI, D. GOUSSIS, F. Creta, AND H. NAJM, *Higher order corrections in the approximation of low-dimensional manifolds and the construction of simplified problems with the CSP method*, *J. Comp. Phys.* 209(2005), 754–786.
- [46] G.J.B. VAN DEN BERG, J. MIRELES-JAMES, *Parameterization of slow-stable manifolds and their invariant vector bundles: theory and numerical implementation*, *DCDS-A*(2016), 4637–4664.
- [47] M. WECHSELBERGER, *Geometric singular perturbation theory beyond the standard form*, *Frontiers in Applied Dynamical Systems* (to appear), Springer, 2019.
- [48] WOLFRAM RESEARCH, INC., *Mathematica, Version 11.1.1.0*, Champaign, IL (2018).

A The formalism underlying the CSP method

The purpose of this section is to collect a few results given across the three very detailed papers [16, 17, 19].

A.1 Change of variables and Lie bracket

In this section, we justify the statement that the variational equation of the transformed vector field has the structure of a Lie bracket as shown in (24)–(25). Differentiating $BA = I$ with respect to t , we obtain the identity

$$BA' = -AB'. \quad (61)$$

Furthermore, the chain rule gives

$$\begin{aligned} A' &= (DA)z' \\ &= (DA)H. \end{aligned} \quad (62)$$

Using identities (61)–(62), the variational equation of the transformed vector field f becomes:

$$\begin{aligned} f' &= (BH)' \\ &= B'H + BH' \\ &= B'Af + B(DH)H \\ &= -BA'f + B(DH)Af \\ &= B(-(DA)Hf + (DH)Af) \\ &= B(-(DA)H + (DH)A)f \\ &= B[A, H]f. \end{aligned} \quad (63)$$

This calculation appears in [19].

A.2 Block-diagonalization of Λ

In this section, we justify the characterizations of the invariant manifold and transverse fiber bundle in terms of a cleverly chosen basis, as shown in (27)–(28). In the presence of an invariant manifold having a transverse fiber bundle which is invariant as a family (i.e. the flow maps fibers into fibers), H can be expressed in a basis which block-diagonalizes the operator Λ . This was proven in [16, 17] for the case of a slow manifold having a transverse fast fiber bundle, but the identical argument carries over without distinguishing ‘slow’ versus ‘fast’ components. We demonstrate this for the vanishing of the upper-diagonal block.

Let \mathcal{M} be an invariant manifold with a transverse fiber bundle \mathcal{N} ; i.e., at a point $z \in \mathcal{M}$, we have the following splitting:

$$T_z \mathbb{R}^n = \mathcal{N}_z \oplus T_z \mathcal{M}_z.$$

We write $A = [A_f \ A_s]$, where the columns of the $n \times (n-k)$ matrix $A_f(z)$ form a basis of \mathcal{N}_z and the columns of the $n \times k$ matrix $A_s(z)$ form a basis of $T_z \mathcal{M}$. The corresponding dual basis similarly spans the dual splitting: we have $B = \begin{pmatrix} B_{s\perp} \\ B_{f\perp} \end{pmatrix}$.

Proposition 1 *For the choice of basis A above, we have $\Lambda_{fs} = \mathbb{O}_{n-k,k}$.*

Proof. We have

$$\begin{aligned} \Lambda_{fs} &= B_{s\perp}[A_s, H] \\ &= B_{s\perp}[(DH)A_s - (DA_s)H]. \end{aligned} \tag{64}$$

By invariance, $H \in TM$ for points in \mathcal{M} , and so $B_{s\perp}H = 0$. The directional derivative along A_s must therefore be identically 0 on \mathcal{M} as well. This gives us the following identity:

$$D(B_{s\perp}H)A_s = DB_{s\perp}(H, A_s) + B_{s\perp}(DH)A_s = 0. \tag{65}$$

Here we clarify that $DB_{s\perp}$ is a symmetric bilinear form, and this (matrix) identity is to be understood as taking the standard directional derivative of each column of A_s in turn and concatenating the result into a matrix.

Similarly, we have the trivial identity $B_{s\perp}A_s = 0$ on \mathcal{M} , coming from the dual basis criterion. Differentiating with respect to t and using the chain rule, we obtain

$$\begin{aligned} \frac{d}{dt}(B_{s\perp}A_s) &= D(B_{s\perp}A_s)H \\ &= D(B_{s\perp})(A_s, H) + B_{s\perp}^\perp(DA_s)H = 0. \end{aligned} \tag{66}$$

Subtracting identities (65) from (66) and using the symmetry of the bilinear form, we obtain $\Lambda_{fs} = 0$. \square

The argument for $\Lambda_{sf} = \mathbb{O}_{n-k,k}$ is similar if slightly more involved, using the invariance of the fiber bundle to obtain an identity as above [17].

A.3 Computation of $\Lambda^{(0)}$

In this section, we derive the formulas (44) for the four block-components of $\Lambda^{(0)} = B^{(0)}[A^{(0)}, H]$. These formulas involve the computation of tensor fields such as $DN(\cdot, \cdot) : T\mathbb{R}^n \times \mathbb{R}^{n-k} \rightarrow \mathbb{R}^n$, which may be defined pointwise at fixed basepoints $z \in \mathbb{R}^n$ as follows:

$$DN(v, \alpha) = \sum_{j_2=1}^n \sum_{j_1=1}^{n-k} \frac{\partial N_{ij_1}}{\partial z_{j_2}} \alpha_{j_1} v_{j_2},$$

where $\alpha = (\alpha_1, \dots, \alpha_{n-k}) \in \mathbb{R}^{n-k}$ and $v = (v_1, \dots, v_n) \in T_z\mathbb{R}^n$.

Remark 12 Fix a basepoint $z \in \mathbb{R}^n$. For $v \in T_z\mathbb{R}^n$, it is natural to denote by DNv the linear transformation $DN(v, \cdot) : \mathbb{R}^{n-k} \rightarrow \mathbb{R}^n$. In particular, DNv can be represented by the $n \times (n-k)$ matrix whose i th column is $DN_i v$, and $DNv\alpha = DN(\alpha, v)$.

The observations in Remark 12 are compatible with our columnwise definition of the Lie bracket (Def. 3.1). For any differentiable vector field V on \mathbb{R}^n and test vector $\phi \in \mathbb{R}^{n-k}$ we have

$$[N, V]\phi = DVN\phi - DNV\phi. \quad (67)$$

Furthermore, we recover a version of the product rule when differentiating the vector field $h_0 = Nf$; for any test tangent vector $v \in T_z\mathbb{R}^n$ we have

$$DHv = D(Nf)v = DN(v, f) + NDfv. \quad (68)$$

The tensor field may be extended in the natural way for matrices of size $n \times d$, where $d \geq 1$. For $X \in (T\mathbb{R}^n)^d \times \mathbb{R}^{n-k} \rightarrow \mathbb{R}^n \times \mathbb{R}^d$, we may define

$$[DN[X, \alpha]]_i = DN[X_i, \alpha], \quad (69)$$

where $i = 1, \dots, d$ and the subscript refers to the i th column of the object. The prior two identities (67) and (68) still hold.

We can repeat these constructions for the tensor field $D(Df^\top)^\perp$. With these results in hand, we proceed to compute the four block components:

$$\begin{aligned}
\Lambda_{ff}^{(0)} &= B_{s\perp}^{(0)}[A_f^{(0)}, H] \\
&= (DfN)^{-1}Df(DHN - DNH) \\
&= (DfN)^{-1}Df((NDf + \varepsilon DG)N + DN(f, N) - DN(Nf + \varepsilon G)) \\
&= DfN + \varepsilon(DGN - DNG) + DN(f, N) - DNNf \\
&= DfN + \varepsilon[N, G]
\end{aligned}$$

$$\begin{aligned}
\Lambda_{fs}^{(0)} &= B_{s\perp}^{(0)}[A_s^{(0)}, H] \\
&= (DfN)^{-1}Df((NDf + \varepsilon DG)(Df^\top)^\perp + DN(f, (Df^\top)^\perp) \\
&\quad - D((Df^\top)^\perp)(Nf + \varepsilon G)) \\
&= Q_1 Df([(Df^\top)^\perp, N]f + \varepsilon[(Df^\top)^\perp, G]), \\
&= \varepsilon Q_1 Df([(Df^\top)^\perp, G] - [(Df^\top)^\perp, N]Q_1 DfG)
\end{aligned}$$

$$\begin{aligned}
\Lambda_{sf}^{(0)} &= B_{f\perp}^{(0)}[A_f^{(0)}, H] \\
&= Q_2(N^\perp)^\top(DHN - DNH) \\
&= Q_2(N^\perp)^\top((NDf + \varepsilon DG)N + DN(f, N) - DN(Nf + \varepsilon G)) \\
&= \varepsilon Q_2(N^\perp)^\top([N, G]),
\end{aligned}$$

$$\begin{aligned}
\Lambda_{ss}^{(0)} &= B_{f\perp}^{(0)}[A_s^{(0)}, H] \\
&= Q_2(N^\perp)^\top((NDf + \varepsilon DG)(Df^\top)^\perp \\
&\quad + DN(f, (Df^\top)^\perp) - D((Df^\top)^\perp)(Nf + \varepsilon G)) \\
&= Q_2(N^\perp)^\top([D(Df^\top)^\perp, N]f + \varepsilon[(Df^\top)^\perp, G]). \\
&= \varepsilon Q_2(N^\perp)^\top([(Df^\top)^\perp, G] - [(Df^\top)^\perp, N]Q_1 DfG),
\end{aligned}$$

where we have also used the fact that $f = -\varepsilon(DfN)^{-1}(DfG)$ on $\mathcal{K}^{(0)}$.