Ref: Proceedings of the IFAC Symposium on Nonlinear Control Design, Tahoe, June 1995.

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GEOMETRY OF COMPUTATIONAL SINGULAR PERTURBATIONS

K. D. Mease*

**Mechanical and Aerospace Engineering, University of California, Irvine, California, 92717-3975, U.S.A. Email: kmease@uci.edu*

Abstract. The previously developed Computational Singular Perturbation (CSP) method is presented from a geometric perspective. Connections are made with previous work on the geometric theory of singular perturbations and decoupling transformations for linear time-varying systems. The CSP method facilitates the numerical solution of multiple time-scale initial-value problems for stiff finite-dimensional nonlinear systems. Its advantage over implicit integration methods is that in addition to producing the solution, it produces information useful in developing reduced-order models. Its advantage over the analytical singular perturbation method is that there is no *a priori* requirement for the system to be given in standard form.

Key Words. Singular Perturbations; Time-Scales; Nonlinear Systems.

1. INTRODUCTION

If the behavior of a dynamical system takes place on two or more widely separated time-scales, there is an opportunity for simplified analysis and design. For a linear time-invariant system, both time and frequency domain methods are available to exploit this opportunity. For a nonlinear system, the analytical singular perturbation method is available, but requires the mathematical model to be given in *standard form* (see Kokotovic, Khalil and O'Reilly, 1986). Unfortunately, a systematic and tractable procedure for transforming a model from non-standard form to standard form is not available (see, however, Marino and Kokotovic (1988)).

The objective of the Computational Singular Perturbation (CSP) method, developed by Lam (1986) and Lam and Goussis (1989), is to produce essentially the same results as the analytical singular perturbation method, while not requiring the system model to be given in standard form. The CSP method has been developed for stiff initial-value problems. A major challenge is to extend CSP to other classes of initial- and boundary-value problems. We are particularly interested in boundary-value problems for Hamiltonian systems that arise as necessary conditions for the solution of optimal control problems. In this paper, we interpret CSP using terminology and concepts from differential geometry (Boothby, 1986 and Spivak, 1979)) and the geometric singular perturbation theory of Fenichel (1979). We feel that the geometric interpretation provides a perspective that will guide future efforts to extend CSP to other classes of initial- and boundary-value problems.

2. TWO TIME-SCALE DYNAMICAL SYSTEM

We assume the mathematical model of the system of interest to be a finite dimensional dynamical system of the form

$$\varepsilon \frac{dx}{dt} = X_\varepsilon(x) \tag{1}$$

with $x(t)$ representing a column vector $(x_1, x_2, ..., x_n)^T$ of coordinates for $\mathbb{R}^n$ and X_ε, a family of vector fields parametrized by $\varepsilon \in \mathbb{R}$ and defined on an open subset of $\mathbb{R}^n$ that contains U (defined below). X_ε is assumed to be a smooth function of x and ε with no explicit dependence on t. We also view the system on the fast time-scale $\tau = t/\varepsilon$ where it takes the form

$$\frac{dx}{d\tau} = X_\varepsilon(x) \tag{2}$$

We focus our attention on an open set $U \subset \mathbb{R}^n$ in which the flow of the dynamical system evolves on two time-scales. The small, non-negative parameter ε dictates the amount of separation between the time-scales. The parameter ε can also play the role of a (singular) perturbation parameter that allows the vector field of interest X_ε to be related to the vector field X_0, the latter being easier to analyze.

3. NOTATION AND CONVENTIONS

We make use of geometric concepts. Although these concepts can be expressed in a coordinate-free manner, we will always consider the setting to be the particular representation of $\mathbb{R}^n$ in which the x-coordinates introduced above correspond to an orthonormal coordinate system. Alternative coordinates will be viewed in general as curvilinear coordinates for that same representation of $\mathbb{R}^n$. The reason for this choice is that the CSP method responds to the situation in which a dynamical system model is provided in a particular set of coordinates and one would like to address the question of whether the system can be decomposed on the basis of time-scale separation.

We use the standard inner product $< y, z >= y^T z$ between vectors $y, z \in \mathbb{R}^n$ expressed in x-coordinates. The length of a vector is denoted by $\|x\| =< x, x >^{1/2}$ and the distance between two points $y, z \in \mathbb{R}^n$ is $d(y, z) = \|y - z\|$.

In connection with a nonlinear differential equation, we use "eigenvectors" to refer to n real vector functions of x that form a basis for $\mathbb{R}^n$ for each value of x and that comprise the columns of a matrix that along with its inverse can be used to transform the Jacobian matrix at each point x into real Jordan canonical form.

The following definitions are required (see Fenichel (1979) for more detail). Let M denote the open set $U \times (-\varepsilon_1, \varepsilon_1) \subset \mathbb{R}^{n+1}$, and let $m = (x, \varepsilon)$ denote a point M. Let $\cdot\tau$ denote the flow induced by the vector field $X_\varepsilon \times 0$, i.e., the trajectory passing through m at $\tau = 0$ is at the point $m \cdot \tau$ at the time τ. The notation $m \cdot [\tau_1, \tau_2]$ represents the segment of the trajectory emanating from m at $\tau = 0$ lying between the points $m \cdot \tau_1$ and $m \cdot \tau_2$. For any subset $V \subset M$ and any subset $J \subset \mathbb{R}$, let $V \cdot J = \{m \cdot \tau : m \in V \quad \text{and} \quad \tau \in J\}$. V is positively invariant if $V \cdot [0, \infty) \subset V$, negatively invariant if $V \cdot (-\infty, 0] \subset V$, and invariant if $V \cdot (-\infty, \infty) \subset V$. Consider two subsets V_1 and V_2 of M such that $V_1 \subset V_2$. V_1 is invariant relative to V_2, if for all $m \in V_1$ we have (i) if $\tau \geq 0$ and $m \cdot [0, \tau] \subset V_2$, then $m \cdot [0, \tau] \subset V_1$ and (ii) if $\tau \leq 0$ and $m \cdot [\tau, 0] \subset V_2$, then $m \cdot [\tau, 0] \subset V_1$. A subset V is said to be *locally invariant* if it is invariant relative to some neighborhood of itself. Suppose that $W \subset M$ is locally positively invariant, and let $\{\mathcal{F}(m) : m \in V\}$ be a smooth foliation of W parametrized by $m \in W$. $\{\mathcal{F}(m) : m \in V\}$ is locally positively invariant foliation, if $\mathcal{F}(m) \cdot \tau \subset \mathcal{F}(m \cdot \tau)$ for all $m \in W$ and all $\tau \geq 0$ such that $m \cdot [0, \tau] \subset W$. Similarly, for W locally negatively invariant, $\{\mathcal{F}(m) : m \in W\}$ is a locally negatively invariant foliation, if $\mathcal{F}(m) \cdot \tau \subset \mathcal{F}(m \cdot \tau)$ for all $m \in W$ and all $\tau \leq 0$ such that $m \cdot [\tau, 0] \subset W$.

4. GEOMETRIC SINGULAR PERTURBATION THEORY

Fenichel (1979) has characterized the geometry of a two time-scale system. He begins with the assumption that there exists an n^0-dimensional (sub)manifold of U called $\mathcal{C}_0$ such that

$$X_0(x) = 0 \qquad \forall x \in \mathcal{C}_0 \tag{3}$$

I.e., $\mathcal{C}_0$ is a manifold of equilibrium points for the vector field X_0. The linearization of Eq. (2) is

$$\frac{d}{d\tau}\delta x = DX_0(x)\delta x \tag{4}$$

where DX_0 is the Jacobian mapping and $\delta x \in T_x U$. The Jacobian mapping at a point $x \in \mathcal{C}_0$ has n^0 zero eigenvalues corresponding to the tangent space of $\mathcal{C}_0$; these are called the trivial eigenvalues. For our purposes here, we assume that the remaining $n - n^0$ eigenvalues have nonzero real parts; these are called the nontrivial eigenvalues. The eigenspace E^c_x associated with the trivial eigenvalues, the null space of $DX_0(x)$, is the tangent space of $\mathcal{C}_0$ at the point x, and is denoted by $T_x\mathcal{C}_0$. Under the assumptions on the eigenvalues, there is a unique complement N_x to $T_x\mathcal{C}_0$ at each point $x \in \mathcal{C}_0$, and thus we have the splitting $T_x U = T_x\mathcal{C}_0 \oplus N_x$ at each point $x \in \mathcal{C}_0$. The eigenvectors associated with the nontrivial eigenvalues form a basis for N_x. N_x is itself the direct sum of two invariant eigenspaces E^s_x and E^u_x, of dimensions n^s and n^u where $n^s + n^u = n - n^0$, associated with the nontrivial eigenvalues with negative and positive real parts, respectively. Thus, at each point $x \in \mathcal{C}_0$, we have $T_x U = E^c_x \oplus E^s_x \oplus E^u_x$.

Theorem 1 (Fenichel, 1979) Consider the extended dynamical system

$$\frac{dx}{d\tau} = X_\varepsilon(x) \tag{5}$$

$$\frac{d\varepsilon}{d\tau} = 0 \tag{6}$$

defined on M.

(i) There exist three locally invariant (sub)manifolds of M near a compact set K of $\mathcal{C}_0$: the center manifold $\mathcal{C}$, the center-stable manifold $\mathcal{C}^s$, and the center-unstable manifold $\mathcal{C}^u$. The center manifold $\mathcal{C}$ contains $K \times \{0\}$ and is tangent to E^c_x at each point $(x, 0) \in K \times \{0\}$. $\mathcal{C}^s$ and $\mathcal{C}^u$ are defined similarly with E^c_x replaced by $E^c_x \oplus E^s_x$ and $E^c_x \oplus E^u_x$, resp. There is a neighborhood V of K, where $V \subset M$, such that the positively invariant points of V belong to $\mathcal{C}^s$, the negatively invariant points of V belong to $\mathcal{C}^u$, and the invariant points of V belong to $\mathcal{C}$.

(ii) There is a locally positively invariant stable smooth foliation $\{\mathcal{F}^s(x, \varepsilon) : (x, \varepsilon) \in \mathcal{C}\}$ of $\mathcal{C}^s$ near K, and a locally negatively invariant unsta-

ble smooth foliation $\{\mathcal{F}^u(x,\varepsilon) : (x,\varepsilon) \in C\}$ of C^u near K. $\mathcal{F}^s(x,0)$ is tangent to E^s_x for each $x \in K$, and $\mathcal{F}^u(x,0)$ is tangent to E^u_x for each $x \in K$.

(iii) There are bounds on the rates at which points in C^s are attracted to the center manifold C and points in C^u are repelled from C. Let $k_s < 0$ be larger than the real parts of the nontrivial eigenvalues with negative real parts, for all points in K. Then there is a constant c_s such that if $m_1 \in C$ and $m_2 \in \mathcal{F}^s(m_1)$, then $d(m_1 \cdot \tau, m_2 \cdot \tau) \leq c_s e^{k_s \tau} d(m_1, m_2)$, for all $\tau \geq 0$ such that $m_1 \cdot [0,\tau] \subset C$. Similarly, let $k_u > 0$ be smaller than the real parts of the nontrivial eigenvalues with positive real parts, for all points in K. Then there is a constant c_u such that if $m_1 \in C$ and $m_2 \in \mathcal{F}^u(m_1)$ $d(m_1 \cdot \tau, m_2 \cdot \tau) \leq c_u e^{k_u \tau} d(m_1, m_2)$, for all $\tau \leq 0$ such that $m_1 \cdot [\tau, 0] \subset C$.

The manifolds C, C^s, and C^u are generalizations of the locally invariant manifolds defined for an isolated equilibrium point. Let C_ε, C^s_ε, and C^u_ε denote the constant ε-slices of C, C^s, and C^u. In particular, the previous use of C_0 to denote the n^0-dimensional manifold of X_0 is now clear.

5. SPECIAL COORDINATES AND ASYMPTOTIC EXPANSIONS

The manifolds C, C^s, and C^u and the foliations $\mathcal{F}^s$ and $\mathcal{F}^u$ can be represented locally as graphs of functions of an appropriate set of coordinates. The functions satisfy partial differential equations consistent with the invariance properties of the manifolds and foliations, and can be constructed in the form of asymptotic expansions.

5.1. *Standard Form*

The standard form is by far the most common and best understood starting point for developing asymptotic solutions to singularly perturbed systems. The standard form is

$$\frac{dy}{dt} = g(y,z;\varepsilon) \tag{7}$$

$$\varepsilon\frac{dz}{dt} = h(y,z;\varepsilon) \tag{8}$$

with (y,z) a set of curvilinear coordinates on U and $y = (y_1, y_2, \ldots, y_{n_0})^T$ and $z = (z_1, z_2, \ldots, z_{n-n_0})^T$. For $\varepsilon = 0$, the cross-section of the center manifold C, i.e., the n_0-dimensional equilibrium manifold C_0, is given by $\{(y,z) : h(y,z;0) = 0\}$. In the formal procedure for constructing solutions in the form of asymptotic series in ε, the center manifold C is represented by $z = \psi(y,\varepsilon) = \psi_0(y) + \varepsilon\psi_1(y) + \ldots$, where $h(y,\psi_0(y);0) = 0$. By the implicit function theorem, $\psi_0(y)$ exists provided that $\partial h/\partial z$ is nonsingular at all points on the surface given by $h(y,z;0) = 0$.

The transformation $x = \Theta(y,z)$ required to convert Eq. (1) to standard form imply considerable *a priori* knowledge about the system behavior. Firstly, the dimension $n_0 + 1$ of the center manifold must be known; secondly, the center manifold must be oriented in the (y,z,ε) frame such that it can be represented in the form $z = \psi(y,\varepsilon)$; and thirdly, the ratio $(dz/dt)/(dy/dt)$ should approach infinity as $\varepsilon \downarrow 0$. Further, since the typical starting point is not an ε-explicit form like Eq. 1, the standard form of the associated differential equations requires the identification (or possibly the introduction) of the small parameter ε.

5.2. *Fenichel's Normal Form*

Theorem 2 (Fenichel, 1979) There exists a local normal form near a point $x_0 \in C_0$, described as follows. There exists a coordinate transformation

$$x = \Upsilon(p, q^s, q^u, \varepsilon) \tag{9}$$

with $p \in \mathbb{R}^{n^\circ}$, $q^s \in \mathbb{R}^{n^s}$ and $q^u \in \mathbb{R}^{n^u}$, such that $x_0 = \Upsilon(0,0,0)$ and points on C have the form $(p,0,0,\varepsilon)$, points on C^s have the form $(p,q^s,0,\varepsilon)$ and points on C^u have the form $(p,0,q^u,\varepsilon)$. In these coordinates, the vector field has the form

$$\frac{dp}{d\tau} = P(p,q^s,q^u,\varepsilon) \tag{10}$$

$$\frac{dq^s}{d\tau} = Q^s(p,q^s,q^u,\varepsilon) \tag{11}$$

$$\frac{dq^u}{d\tau} = Q^u(p,q^s,q^u,\varepsilon) \tag{12}$$

with the following properties. The invariance of C dictates that

$$Q^s(p,0,0,\varepsilon) = 0 \tag{13}$$

$$Q^u(p,0,0,\varepsilon) = 0 \tag{14}$$

$$\frac{\partial Q^s}{\partial p}(p,0,0,\varepsilon) = 0 \tag{15}$$

$$\frac{\partial Q^u}{\partial p}(p,0,0,\varepsilon) = 0 \tag{16}$$

and the normally hyperbolic nature of C (our assumption) dictates that

$$\sigma\left(\frac{\partial Q^s}{\partial p}(p,0,0,0)\right) \in \mathbb{C}^- \tag{17}$$

$$\sigma\left(\frac{\partial Q^u}{\partial p}(p,0,0,0)\right) \in \mathbb{C}^+ \tag{18}$$

where $\sigma()$ denotes the spectrum (set of eigenvalues) of the argument and $\mathbb{C}^-$ and $\mathbb{C}^+$ denote the open left and right-halves of the complex plane. The invariance properties of C^s and $\mathcal{F}^s$ dictate

respectively that

$$Q^u(p, q^s, 0, \varepsilon) = 0 \tag{19}$$

$$\frac{\partial P}{\partial q^s}(p, q^s, 0, \varepsilon) = 0 \tag{20}$$

The invariance properties of $\mathcal{C}^u$ and $\mathcal{F}^u$ dictate respectively that

$$Q^s(p, 0, q^u, \varepsilon) = 0 \tag{21}$$

$$\frac{\partial P}{\partial q^u}(p, 0, q^u, \varepsilon) = 0 \tag{22}$$

6. COMPUTATIONAL SINGULAR PERTURBATIONS

The CSP method aims to achieve the same ends as the analytical singular perturbation method—reduced-order models, approximate solutions, and physical insight—without requiring the system model to be in standard form, or even in the more general, ε-explicit form of Eq. (2). Thus, we now consider a system model of the form

$$\frac{dx}{d\tau} = f(x) \tag{23}$$

on the open set $U \subset \mathbb{R}^n$. Since we are referring to the same underlying system as before, $f(x)$ is a member of the family X_ε for some particular nonzero value of ε denoted by ε_0. Specifically, let $f = X_{\varepsilon_0}$ with $0 < \varepsilon_0 < \varepsilon_1$. The structure of the flow must, however, be deduced without recourse to the $\varepsilon = 0$ limit. Our use of τ rather than t is only a convenience for connecting the subsequent discussion to the preceding theory; it does not imply that we need to know ε_0, since we could have as well used t and identified f with $\frac{1}{\varepsilon_0} X_{\varepsilon_0}$.

The basic idea of CSP is to deduce the two time-scale structure from the size of the fast components of the system vector field. Given the invariance of $\mathcal{C}_{\varepsilon_0}$, $\mathcal{C}^s_{\varepsilon_0}$ and $\mathcal{C}^u_{\varepsilon_0}$ with respect to the flow, at points on these manifolds, $f(x)$ should lie in the respective tangent spaces $T_x\mathcal{C}_{\varepsilon_0}$, $T_x\mathcal{C}^s_{\varepsilon_0}$ and $T_x\mathcal{C}^u_{\varepsilon_0}$. One way to represent T_xU and important subspaces such as $T_x\mathcal{C}_{\varepsilon_0}$ is to use a special set of basis vectors.

6.1. *Special Tangent Space Basis Vectors*

The orthonormal basis for the state space $\mathbb{R}^n$ induces a corresponding orthonormal basis for $T_x\mathbb{R}^n$. A tangent vector, in this basis, has coordinates $\delta x = (\delta x_1, \delta x_2, ..., \delta x_n)^T$. Consider an alternative set of unit basis vectors $\{a_i(x), i = 1, ..., n\}$, not necessarily orthogonal, that span $T_x\mathbb{R}^n$ at each point $x \in U$ and that are smooth functions of x. Each a_i represents a column vector of coordinates with respect to the induced orthonormal basis for $T_x\mathbb{R}^n$. A vector $\delta x \in T_x\mathbb{R}^n$ can be written as

$$\delta x = \sum_{i=1}^{n} a_i(x) v_i \tag{24}$$

in the alternative basis. Henceforth, v will denote the column vector of coordinates $v_1, v_2, ..., v_n$ for a tangent vector with respect to the alternative basis. Note that, if $a_1 = (1, 0, ..., 0)^T, a_2 = (0, 1, 0, ..., 0)^T$, etc., then $v_i = \delta x_i$. We also define $A = col(a_1, ..., a_n)$ and $B = A^{-1}$, so we can write for example that $\delta x = Av$ and $B\delta x = v$.

A distribution on a manifold M is a mapping $\Delta : M \to TM$ defining at each point $m \in M$ a subspace $\Delta(m)$ of the tangent space T_mM. We can define various distributions as the span of various combinations of the basis vectors. In particular, corresponding to Fenichel's local manifold coordinates (p, q^s, q^u), there are the distributions

$$\Delta^p(x) = colspan\ A^p(x) \tag{25}$$

$$\Delta^{q^s}(x) = colspan\ A^{q^s}(x) \tag{26}$$

$$\Delta^{q^u}(x) = colspan\ A^{q^u}(x) \tag{27}$$

where

$$A^p = col\{\partial\Upsilon/\partial p_i / \|\partial\Upsilon/\partial p_i\|, i = 1, \ldots, n^o\}$$

$$A^{q^s} = col\{\partial\Upsilon/\partial q^s_i / \|\partial\Upsilon/\partial q^s_i\|, i = 1, \ldots, n^s\}$$

$$A^{q^u} = col\{\partial\Upsilon/\partial q^u_i / \|\partial\Upsilon/\partial q^u_i\|, i = 1, \ldots, n^u\}$$

I.e., the unitized columns of the Jacobian matrix for the transformation Υ serve as the basis vectors. At each point $x \in U$ we have

$$T_xU = \Delta^p(x) \oplus \Delta^{q^s}(x) \oplus \Delta^{q^u}(x) \tag{28}$$

Using the transformation Υ to local manifold coordinates (p, q^s, q^u) and Eqs. (10-12), we have

$$\frac{dx}{d\tau} = f(x) = A^p P + A^{q^s} Q^s + A^{q^u} Q^u \tag{29}$$

Defining the composite matrix $A = (A^p, A^{q^s}, A^{q^u})$ and separating $B = A^{-1}$ into the row blocks B^p, B^{q^s} and B^{q^u} corresponding to the column blocks of A, we can write

$$P = B^p(x) f(x) \tag{30}$$

$$Q^s = B^{q^s}(x) f(x) \tag{31}$$

$$Q^u = B^{q^u}(x) f(x) \tag{32}$$

Moreover, from Eqs. (13,14,19,21) we obtain the rules

$$x \in \mathcal{C}_{\varepsilon_0} \Rightarrow B^{q^s}(x) f(x) = 0 \tag{33}$$

$$B^{q^u}(x) f(x) = 0 \tag{34}$$

$$x \in \mathcal{C}^s_{\varepsilon_0} \Rightarrow B^{q^u}(x) f(x) = 0 \tag{35}$$

$$x \in \mathcal{C}^u_{\varepsilon_0} \Rightarrow B^{q^s}(x) f(x) = 0 \tag{36}$$

as means of identifying points on $\mathcal{C}_{\varepsilon_0}$, $\mathcal{C}^s_{\varepsilon_0}$ and $\mathcal{C}^u_{\varepsilon_0}$.

With knowledge of the transformation Υ, it is straightforward to determine special basis vectors. Unfortunately it is not straightforward to determine Υ. The CSP method aims to determine special basis vectors directly, without first determining a state transformation such as Υ.

Definition 1. A set of smooth basis vectors $\{a_i(x), i = 1, \ldots, n\}$ for $T_x\mathbb{R}^n$ that has the property

$$\Delta^p(x) = span\{a_1(x), \ldots, a_{n^o}(x)\} \quad (37)$$
$$\Delta^{q^s}(x) = span\{a_{n^o+1}(x), \ldots, a_{n^o+n^s}(x)\} \quad (38)$$
$$\Delta^{q^u}(x) = span\{a_{n^o+n^s+1}(x), \ldots, a_n(x)\} \quad (39)$$

with each distribution involutive, is a modal set and its elements are *modal basis vectors.*

Remark. Modal basis vectors need not correspond to exact differentials of a coordinate transformation as in Eqs. (25-27).

6.2. *Determining Modal Basis Vectors at Points on* $\mathcal{C}_{\varepsilon_0}$

We first make the observation that, in the case $\varepsilon_o = 0$, i.e., $f(x) = X_o$, the eigenvectors of $f_x(x) = \frac{\partial f}{\partial x}(x)$ qualify as modal basis vectors. For the general two time-scale case where $\varepsilon_0 \neq 0$, the points $x \in \mathcal{C}_{\varepsilon_0}$ are not equilibria when viewed on the fast time scale, so the eigenvectors of $f_x(x)$ do not qualify as modal basis vectors. The CSP method is, however, based on:

Assumption 1. At each $x \in \mathcal{C}_{\varepsilon_0}$, the numbers of eigenvalues of $f_x(x)$ with small modulus, large negative and large positive real parts indicate the dimensions n^o, n^s and n^u of the manifolds $\mathcal{C}_{\varepsilon_0}$, $\mathcal{C}^s_{\varepsilon_0}$ and $\mathcal{C}^u_{\varepsilon_0}$.

Assumption 2. At each $x \in \mathcal{C}_{\varepsilon_0}$, the eigenspaces E^o_x, E^s_x and E^u_x, of $f_x(x)$ for "frozen" x, provide approximations to $T_x\mathcal{C}_{\varepsilon_0}$, $T_x\mathcal{C}^s_{\varepsilon_0}$ and $T_x\mathcal{C}^u_{\varepsilon_0}$.

For points $x \in \mathcal{C}_{\varepsilon_0}$, we define the following distributions

$$\hat{\Delta}^p(x) = span\{e^o_1(x), \ldots, e^o_{n^o}(x)\} \quad (40)$$
$$\hat{\Delta}^{q^s}(x) = span\{e^s_1(x), \ldots, e^s_{n^s}(x)\} \quad (41)$$
$$\hat{\Delta}^{q^u}(x) = span\{e^u_1(x), \ldots, e^u_{n^u}(x)\} \quad (42)$$

as approximations of Δ^p, Δ^{q^s} and Δ^{q^u}, where $e^o_i(x)$, $e^s_j(x)$ and $e^u_k(x)$ are the unitized eigenvectors corresponding to E^o_x, E^s_x and E^u_x. Maas and Pope (1992) have in fact used these approximations as a means of locating the slow manifold. In the CSP method, the approximations are refined (when possible, as detailed later) based on the invariance conditions

$$x \in \mathcal{C}_{\varepsilon_0} \quad \Rightarrow \quad [\Delta^p, f] \in \Delta^p \quad (43)$$
$$x \in \mathcal{C}^s_{\varepsilon_0} \quad \Rightarrow \quad [\Delta^{q^s}, f] \in \Delta^{q^s} \quad (44)$$
$$x \in \mathcal{C}^u_{\varepsilon_0} \quad \Rightarrow \quad [\Delta^{q^u}, f] \in \Delta^{q^u} \quad (45)$$

where $[\cdot, \cdot]$ denotes the Lie bracket. The notation $[\Delta, f] \in \Delta$ is shorthand for $[v, f] \in \Delta$, $\forall v \in \Delta$. It is sufficient to check the invariance conditions for the basis vectors of the appropriate distribution.

6.2.1. *Variational Equations.* In the original development of the CSP method (see Lam Refs.), the focus was on a particular state trajectory of the vector field f, the image of the function $\gamma : [0, T] \rightarrow U \subset \mathbb{R}^n$. The evolution of a tangent vector, expressed in the coordinates induced by the x-coordinates, along a trajectory $\gamma(\cdot)$ of Eq. (23) is according to the variational equation

$$\frac{d}{d\tau}\delta x = f_x(\gamma(\tau))\delta x \quad (46)$$

The variational equation along $\gamma(\cdot)$ for the tangent vector coordinates with respect to the alternative basis is

$$\frac{dv}{d\tau} = \left(Bf_xA - B\frac{dA}{d\tau}\right)v = \Lambda(x)v \quad (47)$$

where $A = col(a_i, i = 1, \ldots, n)$ and $B = A^{-1}$ as before except that here the basis vectors are general. The combination of Eqs. (23) and (47) can be viewed specifying a vector field on the tangent bundle $TU = \cup_{x \in U} T_x\mathbb{R}^n$. For a particular set of basis vectors, $a_i(x), i = 1, ..., n$, the matrix Λ can be computed, and the integration of Eq. (23) and Eq. (47) allows the components of a tangent vector in the directions of the chosen basis vectors to be monitored along a state trajectory. The particular tangent vector of interest is $f(x)$.

Consider the case where $\gamma(\cdot)$ lies on the slow manifold $\mathcal{C}_{\varepsilon_0}$. Since the slow manifold is invariant, we must have $f(\gamma(\tau)) \in T_{\gamma(\tau)}\mathcal{C}_{\varepsilon_0}$ at each point of $\gamma(\cdot)$. Now consider a set of modal basis vectors. In such a basis, a vector $v \in T_x\mathcal{C}_{\varepsilon_0}$ has the form $(v_1, \ldots, v_{n^o}, 0, \ldots, 0)^T$; a vector $v \in \Delta^{q^s} \oplus \Delta^{q^u}$ has the form $(0, \ldots, 0, v_{n^o+1}, \ldots, v_n)^T$. The matrix Λ has an $n^o \times n^o$ block corresponding to the slow dynamics and an $(n^s + n^u) \times (n^s + n^u)$ block corresponding to the combined stable and unstable fast dynamics along its diagonal. The off-diagonal coupling blocks of Λ must be zero blocks at each point along $\gamma(\cdot)$, in order that vectors in $T\mathcal{C}_{\varepsilon_0}$ cannot be mapped into vectors in $\Delta^{q^s} \oplus \Delta^{q^u}$ and vice-versa, in accordance with the invariance properties. Note that the Lie bracket of a vector $a(x) \in \Delta^p(x)$ and $f(x)$ is $[a(x), f(x)] = f_xa - a_xf = f_xa - \frac{da}{d\tau}$ and that $[a(x), f(x)] \in \Delta^p(x)$ implies $bf_xa - b\frac{da}{d\tau} = 0$ for all row vectors $b(x) \in B^{q^s} \cup B^{q^s}$, the annihilators of vectors in $\Delta^p(x)$. The elements of the lower off-diagonal block of Λ are all of the form $bf_xa - b\frac{da}{d\tau}$, so zeroing out this block is equivalent to imposing the invariance condition (43). Similarly, the equivalence of zeroing the upper off-

diagonal block with conditions (44) and (45) can be established.

Note that, if the eigenvectors of f_x vary along $\gamma(\cdot)$, the general case, the eigenvectors are not modal basis vectors. Although the eigenvectors block diagonalize the Bf_xA term in Λ, they in general yield nonzero off-diagonal blocks in the $B(dA/d\tau)$ term. The eigenvectors provide a good approximation to modal basis vectors when the off-diagonal blocks of $B(dA/d\tau)$ are small. One means of reducing $B(dA/d\tau)$ is to use basis vectors of unit length, so that $(dA/d\tau)$ only reflects changes in basis vector orientation. Also since the fundamental objects are distributions, not the basis vectors that generate them, there may be basis vectors that span the eigenspaces of interest that change orientation more slowly with x than the eigenvectors, e.g., Schur vectors. Further study of this issue is needed.

6.2.2. *Lyapunov Transformation.* At points on the slow manifold C_{ε_0} we assume that, by using the eigenvectors of f_x along $\gamma(\cdot)$ as the basis vectors, such that the eigenvectors associated with the n^o "small" eigenvalues are taken as the first n^o basis vectors, the variational Eq. (47) takes the form

$$\frac{d}{d\tau}\begin{pmatrix} v^p \\ v^q \end{pmatrix} = \begin{pmatrix} \varepsilon\Lambda_{11} & \varepsilon\Lambda_{12} \\ \Lambda_{21} & \Lambda_{22} \end{pmatrix}\begin{pmatrix} v^p \\ v^q \end{pmatrix} \tag{48}$$

where $v^p = (v_1, ..., v_{n^o})$ and $v^q = (v_{n^o+1}, ..., v_n)$. In particular, we assume that the upper off-diagonal block of $B(dA/dt)$ is small in magnitude. The small parameter ε is shown explicitly for the theoretical development, but is not required for application of the theory. With the variational equation in this form, modal basis vectors can be computed by an iterative procedure for finding a Lyapunov transformation of the tangent vector coordinates that block diagonalizes the transformed Λ matrix in the desired manner. The Lyapunov transformation is of the form

$$\begin{pmatrix} v^{p'} \\ v^{q'} \end{pmatrix} = T_L\begin{pmatrix} v^p \\ v^q \end{pmatrix}$$
$$= \begin{pmatrix} I_{n^o} - \varepsilon N(\tau)L(\tau) & -\varepsilon N(\tau) \\ L(\tau) & I_{n^s+n^u} \end{pmatrix}\begin{pmatrix} v^p \\ v^q \end{pmatrix} \tag{49}$$

where the "prime" denotes the transformed coordinates. If the matrices $L(\tau)$ and $\varepsilon N(\tau)$ are chosen to satisfy the equations

$$\frac{dL}{d\tau} = (\Lambda_{22}L - \Lambda_{21}) - L(\varepsilon\Lambda_{11} - \varepsilon\Lambda_{12}L) \tag{50}$$

$$-\varepsilon\frac{dN}{d\tau} = (\varepsilon N\Lambda_{22} - \varepsilon\Lambda_{12}) + \varepsilon NL\varepsilon\Lambda_{12} - (\varepsilon\Lambda_{11} - \varepsilon\Lambda_{12}L)\varepsilon N \tag{51}$$

then the variational equations in the transformed coordinates are

$$\frac{dv'}{d\tau} = \begin{pmatrix} \varepsilon\Lambda_{11} - \varepsilon\Lambda_{12}L & 0 \\ 0 & \Lambda_{22} - \varepsilon L\Lambda_{12} \end{pmatrix} v' \tag{52}$$

where $v' = (v^{p'}, v^{q'})^T$. The desired block-diagonal structure is thus obtained. The following theorem states the conditions under which the Lyapunov transformation exists and can be determined by an iterative means of computing L and εN.

Theorem 3 (Kokotovic *et al.*, 1986) If (i) Re $\lambda[\Lambda_{22}(\tau)] \leq -c_1 < 0 \quad \forall\tau \in [0,T]$, (ii) the $\Lambda_{ij}(\tau)$ are continuously differentiable and bounded on $[0,T]$, (iii) $\dot{\Lambda}_{12}(\tau), \dot{\Lambda}_{21}(\tau)$, and $\dot{\Lambda}_{22}(\tau)$ are bounded on $[0,T]$, then there exists an $\varepsilon^* > 0$ such that for all $\varepsilon \in (0,\varepsilon^*)$ there are continuously differentiable matrices L and εN, bounded on $[0,T]$, satisfying Eqs. (50) and (51). Moreover,

$$L(\tau) = \Lambda_{22}^{-1}(\tau)\Lambda_{21}(\tau) + O(\varepsilon) \tag{53}$$

$$\varepsilon N(\tau) = \varepsilon\Lambda_{12}(\tau)\Lambda_{22}^{-1}(\tau) + O(\varepsilon^2) \tag{54}$$

The set of modal basis vectors corresponding to the transformed tangent vector coordinates are the columns of A' where

$$A' = AT_L^{-1} \tag{55}$$

and T_L is the Lyapunov transformation matrix. The CSP procedure for determining a set of modal basis vectors follows from the above results. The recursive formula for computing the modal basis vectors is

$$A_{k+1} = A_k(T_L)_k^{-1} \qquad k = 1, 2, \ldots \tag{56}$$

where A_1 is the matrix whose columns are the eigenvectors of f_x ordered with the n^o slow directions preceding the $n^s + n^u$ fast directions and $(T_L)_k$ is the leading order approximation to the Lyapunov transformation matrix in Eq. (49) using the blocks from

$$\Lambda_k = B_k f_x A_k - B_k(\frac{dA}{dt})_k \tag{57}$$

and Eqs. (53) and (54) with ε set to unity. Each column of A_{k+1} should then be unitized. For some low-order systems, the recursive procedure can be carried out symbolically. Otherwise, it is carried out numerically; this requires an approximation for the time rate of change of the A matrix along $\gamma()$.

The modal basis vector computation procedure has its antecedents in the work on decoupling transformations by Chang (1969, 1972) and Kokotovic *et al.* (1975, 1980). Note that *Theorem 3* requires the number of unstable fast modes n^u to be zero (Condition (i)). Refining basis vectors beyond the eigenvector approximations when

$n^u \neq 0$ and at points on $C^s_{\varepsilon_0}$ and $C^u_{\varepsilon_0}$ are topics of current research.

7. APPLICATION OF CSP TO STIFF INITIAL-VALUE PROBLEMS

In the two time-scale case, a stiff initial-value problem is the problem of integrating Eq. (23) from a specified initial condition in the special case of $n^u = 0$, i.e., the slow manifold C_{ε_0} is attracting for all initial conditions in U. An explicit integration method is normally ill-suited for a stiff problem because the integration step must be small enough to follow the fast behavior, even after the fast behavior has died out. An implicit method, such as Gear's, can efficiently integrate the stiff problem, but yields no insight as to the underlying geometric structure. The CSP method operates in conjunction with an integration algorithm which may be explicit, and therefore usually is. At each integration step, or perhaps less often, the eigenvalues and eigenvectors of the Jacobian matrix f_x are computed. The component of the rate of change of the state $\frac{dx}{d\tau} = f(x)$ in the fast eigenspace is computed. At the point where the magnitude of the change in the state due to the fast component of $f(x)$ over the subsequent time step is negligible, the trajectory is in the neighborhood of the slow manifold C_{ε_0}. The refinement (Lyapunov transformation) procedure is activated in order to compute modal basis vectors. Using the (approximate) modal basis vectors, the fast component of $f(x)$ is monitored. When it is sufficiently small, the subsequent integration proceeds as follows. The fast component of $f(x)$ is eliminated by projecting $f(x)$ onto $T_x C_{\varepsilon_0}$, using the projector $A^p B^p$ (see Eqs. (29,30)). The modified vector field is then used in the integration. The integration step can thus be larger – it need only be small enough to follow the slow dynamics. The property that the fast components of $f(x)$ are zero on C_{ε_0} provides n^s approximate integrals of the motion $B^{q^s}(x)f(x) = 0$, that should be satisfied during the subsequent integration and can be used to improve the accuracy of the integration if necessary. These approximate integrals also contain information for constructing reduced-order models.

8. CONCLUSIONS

The Computational Singular Perturbation (CSP) method, developed by Lam, has been interpreted geometrically. Connections have been made with previous work on the geometric theory of singular perturbations and decoupling transformations for linear time-varying systems. The extension of CSP to other classes of initial- and boundary-value problems is the next challenge.

9. ACKNOWLEDGMENT

This research was sponsored by the National Science Foundation. Discussions with Prof. S.-H. Lam, Princeton University, stimulated this research and were crucial to the author's understanding of the computational singular perturbation method.

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