SINGULAR CONTROL-INVARIANCE PDEs
FOR NONLINEAR SYSTEMS[*]

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Abstract. In the present study a new method is proposed that allows the derivation of control laws capable of enforcing the desirable dynamics on an invariant manifold in state space. The problem of interest naturally surfaces in broad classes of physical and chemical systems whose dynamic behavior needs to be controlled and favorably shaped by external driving forces. In particular, the formulation of the problem under consideration is mathematically realized through a system of first-order quasi-linear singular invariance partial differential equations (PDEs), and a rather general set of conditions is derived that ensures the existence and uniqueness of a solution. The solution to the above system of singular PDEs is proven to be locally analytic, thus allowing the development of a series solution method that is easily programmable with the aid of a symbolic software package. Furthermore, through the solution to the above system of singular PDEs, an analytic manifold and a nonlinear control law are computed that render the manifold invariant for the nonlinear dynamical system considered. In particular, the restriction of the system dynamics on the invariant manifold is shown to represent exactly the desirable target dynamics of the controlled system. Finally, an illustrative case study of molecular dissociation is considered, and the proposed method is evaluated through simulation studies.

Key words. invariant manifolds, model reduction, singular partial differential equations, nonlinear dynamics, nonlinear control

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1. Introduction and examples. In recent years, the scientific community has witnessed a resurgence of interest in the challenging problem of controlling the dynamics of nonlinear physical/(bio)chemical systems and processes [1, 2, 3, 4]. Most of these systems/processes exhibit nonlinear dynamic behavior which is typically modeled by systems of nonlinear ordinary differential equations (ODEs) and/or partial differential equations (PDEs) [2, 4, 5, 6]. In particular, it should be pointed out that the practical need to address infinite-dimensional problems, where systems exhibit spatio-temporal characteristics, precipitated a wave of considerable research directed towards the development of computationally efficient dynamic model-reduction techniques [2, 7]. The main idea is the derivation of an accurate approximation of the original infinite-dimensional system by a finite-dimensional one that is mathematically realized by a finite number of ODEs [7]. Early attempts focused on the development of spatial discretization schemes by employing finite-difference or finite-element techniques [2, 7], followed by more elaborate schemes that take into account the classification of PDE systems into hyperbolic or parabolic ones on the basis of the eigenstructure of the spatial differential operator [2, 7]. In particular, for hyperbolic convection-reaction systems that are not amenable to a form of modal decomposition, the method of characteristics has been employed [8]. In the case of parabolic diffusion-reaction systems, the

eigenspectrum of the spatial differential operator exhibits time-scale multiplicity and can be partitioned into a finite-dimensional "slow" part and an infinite-dimensional stable and "fast" complement. An immediate consequence is that the system dynamics is practically determined by only a finite number of "slow" eigenmodes [2, 9]. Computationally efficient modal decomposition techniques such as proper orthogonal decomposition, Karhunen–Loève expansion methods, Galerkin methods, and other sophisticated "hybrid" schemes have also appeared in the pertinent body of literature [2, 10, 11, 12]. Note that the fundamental underlying idea in systems control is the derivation of control laws that appropriately modify and favorably shape the system dynamics, so that a set of prespecified performance objectives are met [6, 13]. One of the most interesting approaches is conceptually aligned with the intuitively appealing idea of the synthesis of control laws capable of rendering a certain manifold invariant in state space, in the sense that the restriction of the system dynamics on the manifold of interest represents the target (desired) dynamics of the controlled system [6, 14, 15]. As a result, the aforementioned performance objectives would be naturally realized through the specific structure of the postulated target dynamics for the controlled system. Even though the notion of invariant manifold successfully serves the purpose of characterizing the dynamic behavior of complex systems through a dimensionality reduction and multiple time-scale analysis, and thus becoming a powerful analytical tool (a representative and certainly not exhaustive sample of recent important contributions can be found in [16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32]), the problem under consideration exhibits a fundamentally different conceptual structure: the invariant manifold of interest is explicitly assigned by the control law derived to the system dynamics in such a manner that the controlled system dynamics (dynamics induced by the control law) represents exactly the desirable target dynamics on the invariant manifold of interest. Therefore, within the proposed framework, the invariant manifold becomes a control law synthesis tool [14, 15]. It should be mentioned that the problem under consideration has been thoroughly addressed for linear systems [33]. In the case of nonlinear systems, however, notable existing approaches in the literature that used rigorous analysis and resulted in theoretically sound results either rely on a set of restrictive conditions or become applicable to special classes of systems [14, 15, 34].

Drawing ample motivation from some preliminary and promising results obtained for linear target dynamics of the controlled system [35], as well as the treatment of the problem under consideration in the discrete-time domain [36], the present research work offers a new approach and methodological perspective that enables the extension of the above results to account for nonlinear target dynamics in the continuous-time domain for the controlled system. The paper is organized as follows: Some necessary mathematical preliminaries, as well as the formulation of the problem of interest, are provided in section 2. The present study's proposed approach and main results derived are presented in section 3, followed by an illustrative case study considered in section 4. Finally, a few concluding remarks are offered in section 5.

2. Mathematical preliminaries: Problem formulation. In the present study nonlinear input-driven dynamical systems are considered:

$$(2.1) \qquad \dot{x} = \frac{dx(t)}{dt} = f(x(t)) + g(x(t))u(t),$$

where t is the time variable, $x \in \mathbb{R}^n$ is the vector of state variables, and $u \in \mathbb{R}$ is the input variable. Without loss of generality, let the origin $x^0 = 0$ be an equilibrium

point of (2.1) that corresponds to $u^0 = 0$: $f(0) = 0$. Indeed, it can be easily inferred that if the reference equilibrium point $P = (x^0, u^0)$ were not zero, then a simple linear invertible coordinate transformation $\bar{x} = x - x^0$, $\bar{u} = u - u^0$ would map P to the origin in the transformed coordinate system $(\bar{x}, \bar{u})$. Note that the lumped-parameter nonlinear dynamic model (2.1) (which serves as our point of departure) could have been obtained via the employment of an appropriate spatial discretization technique applied to the original distributed-parameter dynamic model or any of the available proper orthogonal decomposition, Karhunen–Loève, Galerkin, or other hybrid discretization methods [2, 7]. Indeed, for illustration purposes, let us consider a quasi-linear parabolic diffusion-reaction system modeled by the PDE [2]

$$(2.2) \qquad \frac{\partial v}{\partial t} = A \frac{\partial v}{\partial z} + B \frac{\partial^2 v}{\partial z^2} + b(z)u + f(v)$$

subject to the mixed boundary conditions

$$(2.3) \qquad \begin{aligned} C_1 v(a, t) + D_1 \frac{\partial v}{\partial z}(a, t) &= R_1, \\ C_2 v(b, t) + D_2 \frac{\partial v}{\partial z}(b, t) &= R_2 \end{aligned}$$

and the initial condition

$$(2.4) \qquad v(z, 0) = v_0(z),$$

where $v(z, t) \in \mathbb{R}^n$ is the vector of the state variables, $z \in \Omega = [a, b]$ the spatial coordinate, and $\Omega = [a, b] \subset \mathbb{R}^n$ the spatial domain where the underlying system is defined, and $b(z)$ is a real analytic vector function that describes how the control action $u(t)$ is distributed over the domain Ω. A, B, C_1, D_1, C_2, D_2 are constant matrices, R_1, R_2 are constant vectors of appropriate dimensions, and $v_0(z)$ represents the initial condition which is considered to be known. It is also assumed that $f(v)$ is a real analytic vector function defined on $\mathbb{R}^n$. Let $\mathcal{H} = L^2(\Omega)$ be the Hilbert space consisting of all n-dimensional vector functions defined on Ω and endowed with the inner product and norm [2]

$$(2.5) \qquad \begin{aligned} (v_1, v_2) &= \int_\Omega (v_1(z), v_2(z)) dz, \\ \|v\|_2 &= (v, v)^{1/2} \end{aligned}$$

for all $v_1, v_2 \in \mathcal{H}$, where the symbol $(\cdot, \cdot)$ is used to denote the standard vector inner product in $\mathbb{R}^n$. If one defines the state function $\hat{v}$ on $\mathcal{H}$ as

$$(2.6) \qquad \hat{v}(t) = v(\cdot, t)$$

for all $v \in \mathcal{H}$, the spatial differential operator $\mathcal{A}: H^1(\Omega) \to H^{-1}(\Omega)$ that acts upon vector functions in $H^1(\Omega)$ as follows:

$$(2.7) \qquad \mathcal{A}\hat{v} = A \frac{\partial v}{\partial z} + B \frac{\partial^2 v}{\partial z^2}$$

with

$$(2.8) \quad \hat{v} \in D(\mathcal{A}) = \left\{ \hat{v} \in L^2(\Omega) : \begin{array}{c} \hat{v}, \dfrac{d\hat{v}}{dz} \text{ are abs. continuous, } \dfrac{d^2\hat{v}}{dz^2} \in L^2(\Omega), \\ \text{and } C_i v(a) + D_i \frac{\partial v}{\partial z}(a) = R_i, \ i = 1, 2 \end{array} \right\},$$

and the input operator $\mathcal{B} : U \to H^{-1}(\Omega)$ as

(2.9) $$\mathcal{B}u = b(z)u,$$

then the original PDE system (2.2) assumes the abstract evolution form

(2.10)
$$\dot{\hat{v}} = \frac{d\hat{v}}{dt} = \mathcal{A}\hat{v} + Bu + f(\hat{v}) \qquad \text{in } H^{-1}(\Omega),$$
$$\hat{v}(0) = \hat{v}_0 \in D(\mathcal{A}),$$

where $f(\hat{v}(t)) = f(v(\cdot, t))$ and $\hat{v}_0 = v_0(z)$. It has been observed that for parabolic PDE systems only a few slow dynamic eigenmodes associated with a finite-dimensional part of the eigenspectrum of $\mathcal{A}$ suffice to adequately capture the system's dominant dynamics and therefore allow us to ignore the stable and fast infinite-dimensional complement of $\mathcal{A}$'s eigenspectrum [2]. A standard Galerkin projection of the original PDE system (2.10) on a finite set of eigenfunctions $\{\phi_i,\ i = 1, \ldots, l\}$ associated with the spatial operator $\mathcal{A}$ that correspond to its slow eigenvalues,

(2.11) $$\hat{v} = \sum_{i=1}^{l} a_i(t)\phi_i(z),$$

results in a dynamical system with a state-space representation similar to (2.1). Indeed, in this case the dynamics of the state vector $x = [a_1, \ldots, a_l]$ can be put in the form (see [2])

(2.12) $$\frac{dx}{dt} = f(x) + g(x)u.$$

REMARK 2.1. *If the above partitioning scheme for the eigenspectrum of $\mathcal{A}$ cannot be applied or the eigenfunctions $\{\phi_i\}$ of $\mathcal{A}$ cannot be calculated analytically, one may use empirical eigenfunctions $\{\bar{\phi}_i\}$ [2, 11]. A standard Galerkin projection of the original PDE system* (2.10) *on the aforementioned empirical eigenfunctions,*

(2.13) $$\hat{v} = \sum_{i=1}^{l} \bar{a}_i(t)\bar{\phi}_i(z),$$

results also in dynamics with the state-space representation [2]

(2.14) $$\frac{dx}{dt} = f(x) + g(x)u,$$

where x is now the state vector $x = [\bar{a}_1, \ldots, \bar{a}_l]$.

It should be pointed out that within the context of the present study, classes of Hamiltonian systems that admit the state-space representation (2.1) (such as molecular systems interacting with external electromagnetic fields and modeled in the classical regime) can also be considered. For example, let us for illustration purposes consider a nonrotating chain molecule comprised of $N + 1$ atoms with a field-free Hamiltonian function given by

(2.15) $$H_0(q, p) = \frac{1}{2}p^T G p + V(q),$$

where q is the N-dimensional vector of the bond displacement coordinates, p is the corresponding N-dimensional vector of conjugate momenta, G is the standard Wilson matrix whose elements are associated with the mass of the individual atoms in the molecular chain [37], V is the total potential energy function describing the interactions between the various atoms, and the superscript T is used to denote the transpose of a matrix/vector. The interaction of the molecule with an external laser field is classically described by the Hamiltonian function, assuming that polarization occurs along the molecular chain,

$$(2.16) \qquad\qquad H_I(q) = -\mu(q)\epsilon(t),$$

where $\epsilon(t)$ is the time-dependent external electric field of the laser and $\mu(q)$ the dipole moment function. Therefore, the molecular system's total Hamiltonian function is

$$(2.17) \qquad H(q,p) = H_0(q,p) + H_I(q) = \frac{1}{2}p^T G p + V(q) - \mu(q)\epsilon(t),$$

and the corresponding canonical equations that govern the vibrational molecular motion are given by

$$(2.18) \qquad \begin{aligned} \dot{q}(t) &= \frac{dq}{dt} = \nabla_p H = Gp(t), \\ \dot{p}(t) &= \frac{dp}{dt} = -\nabla_q H = -\nabla_q V(q(t)) + \nabla_q \mu(q(t))\epsilon(t). \end{aligned}$$

Denote by $x = [q,p]^T \in \mathbb{R}^n$ the augmented n-dimensional state $(n = 2N)$ of the molecular motion and $u = \epsilon(t)$ the external laser field. The latter can be viewed as the control/input variable that drives the above canonical equations and can be manipulated according to a certain pattern (control law) in order to modify the system dynamics and achieve dynamic molecular objectives such as dissociation or selective excitation of certain bonds in the molecular chain [3]. Under the above notation, the system of canonical equations (2.18) can be rewritten as an input-driven nonlinear dynamical system that admits the standard state-space representation (2.1) with

$$f(x) = \begin{bmatrix} Gp \\ -\nabla_q V(q) \end{bmatrix} \qquad \text{and} \qquad g(x) = \begin{bmatrix} 0 \\ \nabla_q \mu(q) \end{bmatrix}.$$

Viewing the nonlinear finite-dimensional input-driven dynamical system (2.1) as our point of departure, it is assumed that $f(x), g(x)$ are real analytic vector functions defined on $\mathbb{R}^n$. Moreover, let F be the Jacobian matrix of the vector function $f(x)$ evaluated at the origin,

$$F = \frac{\partial f}{\partial x}(0),$$

and let G be the $n \times 1$ vector $G = g(0)$. The following assumption is also made.

Assumption 2.1. The $(n \times n)$ matrix $\mathcal{C}$ defined via

$$(2.19) \qquad\qquad \mathcal{C} = \begin{bmatrix} G & | & FG & | & \dots & | & F^{n-1}G \end{bmatrix}$$

has rank n: $\mathrm{rank}(\mathcal{C}) = n$.

The primary objective is as follows:

(i) Given a real analytic nonlinear vector function $h : \mathbb{R}^n \to \mathbb{R}^n$ with $h(0) = 0$ and target dynamics for the controlled system

$$(2.20) \qquad \dot{z} = \frac{dz}{dt} = h(z),$$

find an analytic invariant manifold $z = S(x)$ with $S : \mathbb{R}^n \to \mathbb{R}^n$ being a real analytic vector function such that $S(0) = 0$.

(ii) Derive a control law $u = T(z) = T(S(x))$, with $T : \mathbb{R}^n \to \mathbb{R}$ being a real analytic scalar function satisfying $T(0) = 0$, that renders the manifold invariant for the augmented system

$$(2.21) \qquad \begin{aligned} \dot{x} &= f(x) + g(x)T(z), \\ \dot{z} &= h(z), \end{aligned}$$

such that the restriction of the system dynamics (2.21) on the manifold $z = S(x)$ is exactly the target dynamics (2.20).

REMARK 2.2. *At this point let us examine how the postulated nonlinear target dynamics (2.20) emerges in a meaningful molecular dissociation problem. For simplicity, let us consider a diatomic ($N = 2$) molecule in the presence of an external laser field whose motion is described by the system of canonical equations (2.18). In a similar spirit as in [3, 4], a physically meaningful choice for the target z-dynamics (2.20) would be the antidamped oscillator subject to the same potential as the molecule of interest,*

$$(2.22) \qquad \begin{aligned} \dot{q}_d &= \frac{dq_d}{dt} = \frac{p_d}{m}, \\ \dot{p}_d &= \frac{dp_d}{dt} = -\frac{\partial V}{\partial q_d}(q_d) + \frac{ap_d}{m}, \end{aligned}$$

where $a > 0$ is the antidamping constant. Under the above nonlinear target dynamics (2.22) (which may be equivalently represented via the augmented z-state vector $z = [q_d, p_d]^T$ in the form (2.20)), the time derivative of the molecular energy function E_d along the trajectories of the target dynamics (2.22) can be readily calculated and is given by

$$(2.23) \qquad \dot{E}_d = \frac{dE_d}{dt} = \frac{ap_d^2}{m^2} > 0.$$

Note that the above monotonicity property of the dynamic profile of E_d is meaningfully correlated with the molecular dissociation objective and the breaking of the bond between the atoms [3, 4].

Let us now assume that the requisite control law is given by $u = T(z) = -Cz = -CS(x)$, where C is a given constant vector and $S(x)$ the unknown mapping that is associated with the invariant manifold $z = S(x)$. Then the aforementioned invariance requirement can be mathematically translated into the system of first-order quasi-linear PDEs [38, 39]

$$(2.24) \qquad \begin{aligned} \frac{\partial S}{\partial x}\{f(x) - g(x)CS(x)\} &= h(S(x)), \\ S(0) &= 0, \end{aligned}$$

where the vector function $S \in \mathbb{R}^n$ is the unknown solution of (2.24). Note that the above first-order quasi-linear invariance PDEs (2.24) have a common principal part: $f(x) - g(x)CS(x)$. Furthermore, the equilibrium point $x^0 = 0$ is a *characteristic point* for the above system of PDEs (2.24), since the common principal part vanishes at $x^0 = 0$ where $S(0) = 0$, and therefore the system of PDEs (2.24) becomes a *singular* one [40]. Note that in this case any attempt to mathematically characterize the solution properties of the invariance singular PDEs (2.24) in a neighborhood of the characteristic point $x^0 = 0$ (and the present research study focuses on this case) impinges on the fact that the existence and uniqueness conditions of the Cauchy–Kovalevskaya theorem are not satisfied [40], and, as will be seen below, one inevitably needs to rely on methods and results from singular PDE theory [41, 42].

REMARK 2.3. *The proposed method aims at deriving a nonlinear control law that forces the molecular system of interest to follow the prescribed target dynamics (2.20) on the appropriate manifold $S(x)$. Furthermore, the choice of the eigenspectrum of the characteristic Jacobian matrix $A = \frac{\partial h}{\partial z}(0)$ of the target dynamics (2.20) is critical, since it captures the system's desirable dynamic eigenmodes on the manifold. For example, an elementary analysis shows that the antidamping constant a in Remark 2.1 needs to be positive for a meaningful molecular dissociation problem such as the one considered.*

REMARK 2.4. *Consider the augmented system dynamics*

$$(2.25) \qquad \begin{aligned} \dot{x} &= f(x) - g(x)Cz, \\ \dot{z} &= h(z), \end{aligned}$$

which can be viewed as the product of a cascade connection between the autonomous dynamics of the target system

$$(2.26) \qquad \begin{aligned} \dot{z} &= h(z), \\ u &= -Cz \end{aligned}$$

and the original system dynamics

$$(2.27) \qquad \dot{x} = f(x) + g(x)u,$$

being driven by the "output" $u = -Cz$ of the target system (2.26). The augmented system dynamics (2.25) can be mathematically characterized as a skew product system, whose class frequently arises in the study of the dynamic behavior of systems driven by the autonomous dynamics of an exogeneous system [43, 44]. Furthermore, within this context, the graph of the function $z = S(x)$ is a manifold which is rendered invariant by construction (satisfying the system of singular quasi-linear invariance PDEs (2.24)) [38, 39].

3. Main results. The following proposition establishes the requisite set of conditions for the existence and uniqueness of a locally analytic invertible solution of the system of singular PDEs (2.24).

PROPOSITION 3.1. *Consider the system of first-order singular quasi-linear invariance PDEs (2.24). Furthermore, assume the following.*

Assumption 3.1. The $n \times n$ matrix $A = \frac{\partial h}{\partial z}(0)$ has eigenvalues k_i that satisfy the condition

$$(3.1) \qquad 0 \notin \mathbf{co}\{k_1, k_2, \ldots, k_n\},$$

where **co** stands for the convex hull of a set (Poincaré domain [45]).

Assumption 3.2. The eigenspectra $\sigma(A)$, $\sigma(F)$ of matrices A and F, respectively, are disjoint: $\sigma(A) \cap \sigma(F) = \emptyset$.

Assumption 3.3. The eigenvalues k_i of A are not related to the eigenvalues λ_j of F through any equations of the type

$$(3.2) \qquad \sum_{i=1}^{n} m_i k_i = \lambda_j$$

$(j = 1, \ldots, n)$, where all the m_i are nonnegative integers that satisfy the condition

$$(3.3) \qquad \sum_{i=1}^{n} m_i > 1.$$

Assumption 3.4. The pair of matrices (C, A) is chosen such that the following $(n \times n)$ matrix $\mathcal{O}$ defined via

$$(3.4) \qquad \mathcal{O} = \begin{bmatrix} C \\ CA \\ \vdots \\ CA^{n-1} \end{bmatrix}$$

has rank n: $\operatorname{rank}(\mathcal{O}) = n$.

Then the system of first-order singular quasi-linear PDEs (2.24) *with initial condition $S(0) = 0$ admits a unique and locally analytic invertible solution $w = S(x)$ in a neighborhood of the equilibrium point $x^0 = 0$.*

Proof. Let us first denote

$$(3.5) \qquad \begin{aligned} f(x) &= Fx + \bar{f}(x), \\ g(x) &= G + \bar{g}(x), \\ h(z) &= Az + \bar{h}(z), \\ S(x) &= \mathcal{S}x + \bar{S}(x), \end{aligned}$$

with $\frac{\partial \bar{f}}{\partial x}(0) = \frac{\partial \bar{S}}{\partial x}(0) = \frac{\partial \bar{h}}{\partial z}(0) = \bar{g}(0) = 0$.

Under the above notation, the system of invariance PDEs (2.24) becomes

(3.6)
$$\left\{ \mathcal{S} + \frac{\partial \bar{S}}{\partial x} \right\} \{ (F - GC\mathcal{S})x - GC\bar{S} + \bar{f} - \bar{g}C\mathcal{S}x - \bar{g}C\bar{S} \} = A\mathcal{S}x + A\bar{S} + \bar{h}(\mathcal{S}x + \bar{S}).$$

From (3.6) it can be easily inferred that the unknown $(n \times n)$ matrix $\mathcal{S}$ has to satisfy the quadratic matrix equation

$$(3.7) \qquad \mathcal{S}F - A\mathcal{S} = \mathcal{S}GC\mathcal{S}$$

and the unknown vector function $\bar{S}(x)$ the system of first-order quasi-linear singular PDEs

$$(3.8) \qquad \frac{\partial \bar{S}}{\partial x} \{ \tilde{A}x + \Phi(x, \bar{S}) \} = \tilde{F}\bar{S} + \Psi(x, \bar{S}),$$

where

$$
\begin{aligned}
\tilde{A} &= F - GC\mathcal{S}, \\
\tilde{F} &= A + \mathcal{S}GC, \\
\Phi(x, \bar{S}) &= -GC\bar{S} + \bar{f} - \bar{g}C\mathcal{S}x - \bar{g}C\bar{S}, \\
\Psi(x, \bar{S}) &= -\mathcal{S}\bar{f} + \mathcal{S}\bar{g}C\mathcal{S}x + \mathcal{S}\bar{g}C\bar{S} + \bar{h}(\mathcal{S}x + \bar{S}).
\end{aligned}
$$

(3.9)

In (3.9) note that

(3.10)
$$
\Phi(0,0) = \Psi(0,0) = 0
$$

and

(3.11)
$$
\frac{\partial \Psi}{\partial x}(0,0) = 0.
$$

Let us now consider the standard Lyapunov matrix equation

(3.12)
$$
FT - TA = GC.
$$

Under Assumptions 2.1, 3.2, and 3.4, one can prove that the above Lyapunov matrix equation admits a unique and invertible solution T [13, 46]. Furthermore, one can also show that the inverse matrix T^{-1} satisfies the quadratic matrix equation

(3.13)
$$
T^{-1}F - AT^{-1} = T^{-1}GCT^{-1},
$$

which coincides with (3.7), and therefore

(3.14)
$$
\mathcal{S} = T^{-1}.
$$

Moreover, using (3.7) one obtains

$$
\begin{aligned}
F - GC\mathcal{S} &= \mathcal{S}^{-1}A\mathcal{S} = \tilde{A}, \\
A + \mathcal{S}GC &= \mathcal{S}F\mathcal{S}^{-1} = \tilde{F}.
\end{aligned}
$$

(3.15)

Note that from (3.15) it can be inferred that matrices $\tilde{A}, \tilde{F}$ are similar to A, F, respectively, and therefore they have the same set of eigenvalues. At this point Lyapunov's auxiliary theorem is invoked in order to address the issue of the existence and uniqueness of an analytic solution $\bar{S}$ of the system of first-order quasi-linear singular PDEs (3.8).

THEOREM 3.2 (Lyapunov's auxiliary theorem) (see [35, 42]). *Consider the system of first-order quasi-linear partial differential equations*

(3.16)
$$
\begin{aligned}
\frac{\partial w}{\partial x}\phi(x, w) &= \psi(x, w), \\
w(0) &= 0,
\end{aligned}
$$

with

(3.17)
$$
\begin{aligned}
\phi(0,0) &= 0, \\
\psi(0,0) &= 0, \\
\frac{\partial \psi}{\partial x}(0,0) &= 0,
\end{aligned}
$$

where $w \in \mathbb{R}^n$ is the unknown solution of (3.16) and $\phi(x,w) : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^n$ and $\psi(x,w) : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^n$ are analytic vector functions. It is assumed that the eigenvalues k_i $(i = 1, \ldots, n)$ of the $n \times n$ matrix $\frac{\partial \phi}{\partial x}(0,0)$ satisfy the condition

$$(3.18) \qquad 0 \notin \mathbf{co}\{k_1, k_2, \ldots, k_n\},$$

where $\mathbf{co}$ stands for the convex hull of a set, and are not related to the eigenvalues λ_i $(i = 1, \ldots, n)$ of the $n \times n$ matrix $\frac{\partial \psi}{\partial w}(0,0)$ through any equation of the type

$$(3.19) \qquad \sum_{i=1}^{n} m_i k_i = \lambda_j$$

$(j = 1, \ldots, n)$, where all the m_i are nonnegative integers that satisfy the condition

$$(3.20) \qquad \sum_{i=1}^{n} m_i > 1.$$

Then the above system of first-order quasi-linear PDEs (3.16) admits a unique analytic solution $w = S(x)$ in a neighborhood of $x^0 = 0$ with $\frac{\partial w}{\partial x}(0) = 0$.

Under the assumptions of Proposition 3.1, one can conclude that Lyapunov's auxiliary theorem guarantees indeed the existence and uniqueness of an analytic solution $\bar{S}$ of the system of first-order quasi-linear PDEs (3.8) in a neighborhood of $x^0 = 0$. Therefore, we may also easily conclude that the original first-order system of singular quasi-linear invariance PDEs (2.24) admits a unique analytic solution $w = S(x)$ in a neighborhood of $x^0 = 0$, and, since $\mathcal{S}$ is nonsingular, the solution $w = S(x)$ of (2.24) is also locally invertible around $x^0 = 0$. $\quad\square$

REMARK 3.1. *Let us now briefly comment on the set of conditions derived (Proposition 3.1) for the existence and uniqueness of a locally analytic and invertible solution to the system of first-order quasi-linear invariance PDEs (2.24). Assumptions 3.2 and 3.3 and conditions (3.2)–(3.3), which are "nonresonance conditions" imposed on the eigenvalues of the F and A matrices, are needed to prove the existence of a unique formal power-series solution to the system of singular invariance PDEs (2.24) [41, 42]. Assumption 3.1 is indispensable in the proof to show uniform convergence of the above formal power series in a neighborhood of $x^0 = 0$ and the solution's analyticity property [41, 42]. Assumptions 2.1 and 3.4 guarantee the invertibility of matrix $\mathcal{S}$, and thus the local invertibility property of the solution $S(x)$ of the PDEs (2.24) (see the proof of Proposition 3.1 and [13, 46]).*

REMARK 3.2. *In the linear case where $f(x) + g(x)u = Fx + Gu$, $h(z) = Az$, the system of invariance PDEs (2.24) assumes the form*

$$(3.21) \qquad \frac{\partial S}{\partial x}\{Fx - GCS\} = AS.$$

The solution is of the linear form $S = \mathcal{S}x$, where the constant matrix $\mathcal{S}$ has to satisfy the matrix equation

$$(3.22) \qquad \mathcal{S}F - A\mathcal{S} = \mathcal{S}GC\mathcal{S}.$$

The above is exactly (3.7). Under the stated assumptions, and as it has been previously shown, (3.22) admits a unique invertible solution $\mathcal{S}$ [13, 46]. Note that the above solution coincides with the one offered by linear analysis [47], and therefore the

proposed method may be viewed as its nonlinear analogue, since it naturally reproduces the linear result as a special case.

COROLLARY 3.3. *Under the assumptions of Proposition* 3.1, *let* $S(x)$ *be the unique analytic and locally invertible solution of the system of singular quasi-linear invariance PDEs* (2.24) *in a neighborhood of* $x^0 = 0$. *Then the graph of the mapping* $z = S(x)$ *is an analytic manifold which is rendered locally invariant by the feedback control law* $u = -CS(x)$, *and the restriction of the system dynamics* (2.1) *on this manifold is exactly the prescribed target dynamics* (2.20).

Proof. The restriction of the system dynamics (2.1) on the manifold $z = S(x)$ is given by

$$(3.23) \qquad \dot{z} = \frac{\partial S}{\partial x}\dot{x} = \frac{\partial S}{\partial x}\{f(x) - g(x)CS(x))\} = h(S(x)) = h(z).$$

Note that the aforementioned dynamics coincides with the nonlinear target dynamics of the controlled system (2.20), thus completing the proof. $\square$

REMARK 3.3. *Note that it is always possible to select the eigenvalues of matrix A (a design/adjustable parameter) so that* (i) *the resonance conditions* (3.2)–(3.3) *are avoided,* (ii) *the eigenspectra of A and F are disjoint, and* (iii) *the pair of matrices* (C, A) *satisfies the rank condition* (3.4). *Consequently, the assumptions of Proposition* 3.1 *and Corollary* 3.3 *are not restrictive.*

3.1. Series solution of the system of singular quasi-linear invariance PDEs. The development of a comprehensive and practical solution scheme for the system of first-order singular invariance PDEs (2.24) is needed at the implementation stage of the proposed method. It should be noted that the method of characteristics cannot be applied to PDEs (2.24) due to the associated singularity at the origin and the fact that the pertinent theory inevitably breaks down [40]. However, since the real functions $f(x)$, $g(x)$, $h(z)$, as well as the unknown solution $S(x)$ of (2.24), are all locally analytic around the origin, one can (i) expand $f(x)$, $g(x)$, $h(z)$, $S(x)$ in multivariate Taylor series and (ii) equate the Taylor coefficients of the same order for both sides of the invariance PDEs (2.24). This procedure leads to a set of linear recursion formulas, through which one can calculate the Nth order Taylor coefficients of the unknown solution $S(x)$, given the Taylor coefficients of $S(x)$ up to the order $N-1$, that have already been calculated in previous recursive steps. For the derivation of the aforementioned recursion formulas the following convenient tensorial notation is adopted [35]:

(a) The entries of a constant matrix A are represented as a_i^j, where the subscript i refers to the corresponding row and the superscript j to the corresponding column of the matrix.

(b) The partial derivatives of the μth component $f_\mu(x)$ of the vector function $f(x)$ with respect to x evaluated at $x = 0$ are denoted as follows:

$$f_\mu^i = \frac{\partial f_\mu}{\partial x_i}(0,0),$$

$$(3.24) \qquad f_\mu^{ij} = \frac{\partial^2 f_\mu}{\partial x_i \partial x_j}(0,0),$$

$$f_\mu^{ijk} = \frac{\partial^3 f_\mu}{\partial x_i \partial x_j \partial x_k}(0,0),$$

etc.

(c) The standard summation convention is used where repeated upper and lower tensorial indices are summed up.

In light of the above notation, one can represent the lth component $S_l(x)$ of the unknown solution $S(x)$ as a Taylor series:

$$(3.25) \quad S_l(x) = \frac{1}{1!} S_l^{i_1} x_{i_1} + \frac{1}{2!} S_l^{i_1 i_2} x_{i_1} x_{i_2} + \cdots + \frac{1}{N!} S_l^{i_1 i_2 \ldots i_N} x_{i_1} x_{i_2} \ldots x_{i_N} + \cdots .$$

In a similar fashion the vector functions $f(x)$, $g(x)$, $h(z)$ are expanded in Taylor series, and these expansions are then inserted into the invariance PDEs (2.24). Equating the Taylor coefficients of the same order for both sides of (2.24), the following recursive relations are obtained.

First-order terms.

$$(3.26) \qquad\qquad S_l^\mu (f_\mu^{i_1} - g_\mu c^k S_k^{i_1}) = a_l^\mu S_\mu^{i_1}$$

with $i_1 = 1, \ldots, n$ and $l = 1, \ldots, n$. Note that the above set of linear algebraic equations can be recast into the matrix equation (3.7), that is, also obtained from linear analysis.

Nth-order terms.

$$(3.27) \quad \sum_{L=0}^{N-1} \sum_{\binom{N}{L}} S_l^{\mu i_1 \ldots i_L} (f_\mu^{i_{L+1} \ldots i_N} - \pi_\mu^{i_{L+1} \ldots i_N}) = a_l^\mu S_\mu^{i_1 \ldots i_N} + \zeta_l^{i_1 \ldots i_N} (S^{i_1 \ldots i_{N-1}}),$$

where

$$(3.28) \qquad\qquad \pi_\mu^{j_1 \ldots j_M} = \sum_{P=0}^{M-1} \sum_{\binom{M}{P}} g_\mu^{j_1 \ldots j_P} c^k w_k^{j_{P+1} \ldots j_M}$$

$(i_1, \ldots, i_N = 1, \ldots, n; l = 1, \ldots, n)$ with $\zeta_l^{i_1 \ldots i_N} (S^{i_1 \ldots i_{N-1}})$ being a function of Taylor coefficients of the unknown solution $S(x)$ calculated in the previous recursive steps. Note that the second summation symbols in (3.27)–(3.28) suggest summing up the relevant quantities over the $\binom{N}{L}$ and $\binom{M}{P}$ possible combinations of the indices $(i_1, \ldots, i_N)$ and $(j_1, \ldots, j_M)$, respectively. Furthermore, attention should be drawn to the fact that (3.27)–(3.28) represent a set of linear algebraic equations with respect to the unknown coefficients $S_\mu^{i_1 \ldots i_N}$, and that is precisely the reason that the proposed series solution method for the system of invariance PDEs (2.24) becomes amenable to an easy implementation by using a symbolic software package such as MAPLE. In particular, an efficient MAPLE code has been developed to automatically generate the various coefficients of the Taylor series representation of the unknown solution $S(x)$ of the invariance PDEs (2.24).

REMARK 3.4. *It should be pointed out that occasionally the Taylor series solution method for the invariance PDEs (2.24) exhibits slow convergence. In these cases, significant improvement of the convergence properties of the PDE solution scheme can be achieved if direct Newton-type methods as described in [48] are employed or relaxation methods such as the ones reported in [17, 49].*

4. Illustrative example. The problem of using laser pulses to modify the dynamics, and hence the properties, of molecular systems has attracted a lot of attention in recent years, not only due to its theoretical significance but also its potential to revolutionize the fields of nanotechnology, quantum computing, communications safety,

materials processing, etc. [3, 50, 51, 52]. The study of the above problem poses a great challenge in the classical regime and more profoundly in the quantum mechanical regime when formulated as a control problem [3, 50, 51, 52]. Within a control context, the laser field is viewed as the manipulated input variable through which the desirable dynamics is assigned to the molecular system of interest in either an open-loop or closed-loop fashion [3, 50, 51, 52]. Attention should be drawn to the fact that even though the conceptual formulation and formal mathematical treatment of the above problem as a typical control problem is feasible, its study requires the in-depth resolution of an array of challenging issues associated with the actual implementability and physical realizability of the proposed control algorithm/strategy and the associated external laser field, as it interferes with the underlying laws of nature that govern the interaction of matter with light (particularly from a quantum mechanical point of view) [3, 50, 51, 52]. However, recent advances in optics, laser chemistry, and spectroscopy allowed a great deal of progress to be made and a lot of the aforementioned fundamental issues to be addressed in a comprehensive and thorough manner (see [50, 51, 52], as well as references therein, for a representative sample of research results obtained by pioneers in this field). In the context of the present study, and in order to simply illustrate the proposed control method (which is the focus of the paper), the dissociation problem of a diatomic molecule in the presence of an external laser field is considered. In the classical regime, the diatomic molecular system is often modeled as a rotationless oscillator with a Morse potential energy function given by

$$(4.1) \qquad V(q) = D[1 - \exp(-\beta q)]^2,$$

where q is the displacement (spatial) coordinate in the standard two-body problem formulation and D, β are positive constants [37]. In the absence of an external electromagmetic field, the Hamiltonian of the molecular system is given by

$$(4.2) \qquad H_0 = \frac{p^2}{2m} + V(q),$$

where p is the conjugate momentum and m the molecular reduced mass. Whenever the molecule is exposed to an external laser field, the interaction between the molecule and the laser field is described by the Hamiltonian function

$$(4.3) \qquad H_I = -\mu(q)\epsilon(t),$$

where $\epsilon(t)$ is the time-dependent control laser field polarized along the molecular axis, and the dipole moment function $\mu(q)$ is given by

$$(4.4) \qquad \mu(q) = B(q + q_0) \exp[-\gamma(q + q_0)^4],$$

with B, γ, q_0 being positive constants [3]. Let us now denote by $H = H_0 + H_I$ the system's total Hamiltonian function. In the classical Hamiltonian formalism employed, the following system of canonical equations can be obtained:

$$(4.5) \qquad \begin{aligned} \dot{q} &= \frac{\partial H}{\partial p} = \frac{p}{m}, \\ \dot{p} &= -\frac{\partial H}{\partial q} = -\frac{\partial V}{\partial q}(q) + \frac{\partial \mu}{\partial q}(q)\epsilon(t). \end{aligned}$$

In the context of the present study, the primary control objective is to derive a control law $\epsilon(t)$ (or the necessary profile of the external laser field) that will eventually cause the bond of the diatomic molecule to break. In order to achieve the above molecular dissociation objective one would preferably request a control field $\epsilon(t)$ that would induce target dynamics exhibiting "antidamped" behavior, and thus leading to the attainment of energy levels above the dissociation threshold. As mentioned earlier (section 2), a physically meaningful choice for the target dynamics of the controlled system is the antidamped oscillator subject to the same potential as the molecule under consideration,

(4.6)
$$\dot{q}_d = \frac{p_d}{m},$$
$$\dot{p}_d = -\frac{\partial V}{\partial q_d}(q_d) + \frac{a p_d}{m},$$

where $a > 0$ is the antidamping constant. Let us now denote $x_1 = q$, $x_2 = p$, $u = \epsilon$, $z_1 = q_d$, $z_2 = p_d$. Selecting $C = \begin{bmatrix} 0 & 1 \end{bmatrix}$ and using the model parameter values given in [3, 37], all conditions of Proposition 3.1 and Corollary 3.3 are met, and therefore the system of invariance PDEs

(4.7)
$$\frac{\partial S_1}{\partial x_1}\{f_1(x_1, x_2) - g_1(x_1, x_2)S_2(x_1, x_2)\} + \frac{\partial S_1}{\partial x_2}\{f_2(x_1, x_2) - g_2(x_1, x_2)S_2(x_1, x_2)\}$$
$$= h_1(S_1(x_1, x_2), S_2(x_1, x_2)),$$
$$\frac{\partial S_2}{\partial x_1}\{f_1(x_1, x_2) - g_1(x_1, x_2)S_2(x_1, x_2)\} + \frac{\partial S_2}{\partial x_2}\{f_2(x_1, x_2) - g_2(x_1, x_2)S_2(x_1, x_2)\}$$
$$= h_2(S_1(x_1, x_2), S_2(x_1, x_2)),$$
$$S_1(0, 0) = 0,$$
$$S_2(0, 0) = 0$$

admits a unique and locally analytic invertible solution: $S_1(x_1, x_2)$, $S_2(x_1, x_2)$. As mentioned earlier, the above solution can be computed in a Taylor series form using a MAPLE code, and the control law that enforces the nonlinear target dynamics (4.6) on the invariant manifold $z = [z_1, z_2] = S(x_1, x_2) = [S_1(x_1, x_2), S_2(x_1, x_2)]$ is

(4.8)
$$u(t) = -CS(x_1(t), x_2(t)) = -S_2(x_1(t), x_2(t)).$$

A third-order Taylor polynomial approximation of the actual solution of the system of PDEs (4.7) is considered resulting from a third-order series truncation ($N = 3$) of the Taylor series. The following expression for the control law is obtained:

(4.9)
$$u(t) = -S_2(x_1(t), x_2(t)) = 0.00123 x_2(t) - 0.000195 x_1^2(t) + 0.0016 x_1(t)x_2(t)$$
$$- 6 \times 10^{-7} x_2^2(t) - 0.919 x_1^3(t) + 0.0011 x_1^2(t)x_2(t)$$
$$- 0.0008 x_1(t)x_2^2(t) - 5 \times 10^{-7} x_2^3(t).$$

Note that if the linear terms in the above expression (4.9) are singled out, the resulting linear control law matches exactly the one offered by standard linear analysis arguments [47]. When the control law (4.9) is applied to the system, the profile of
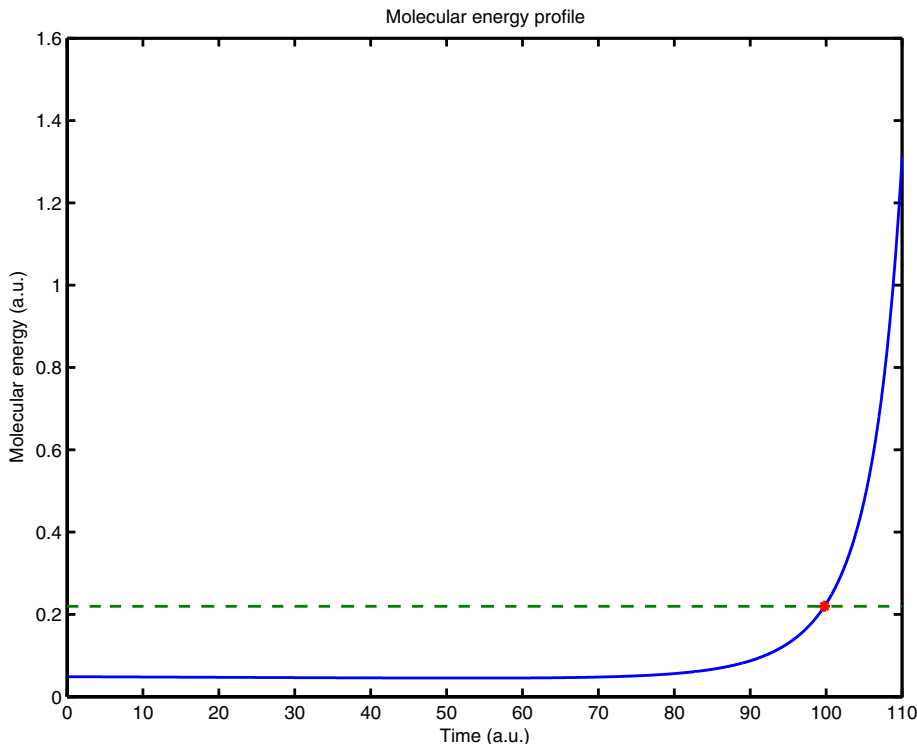
Fig. 1. *Molecular energy profile.*

the molecular energy induced is as graphically depicted in Figure 1, suggesting that the dissociation energy threshold is exceeded, the bond is broken, and the molecular objective is met. The corresponding dynamic profile of the control field applied is presented in Figure 2. Note that during the first stage, relatively mild amounts of energy are being transferred to the molecular system, followed by a second and more intense one, where the energy provision by the laser source suffices for the molecular energy to exceed the dissociation threshold. Finally, it should be pointed out that the academic example considered is meant to illustrate only the key features of the proposed control methodology. Aspects pertaining to the actual implementability, as well as physical realizability of the above control laser field in the lab, while quite important [50, 51, 52], are not addressed in the context of the present study.

5. Concluding remarks. A new method that allows the derivation of control laws capable of enforcing the desirable system dynamics on an invariant manifold in state space was presented. The problem of interest was formulated and addressed within the framework of singular PDE theory. It was proven that through the solution of a system of first-order quasi-linear singular PDEs a locally analytic manifold can be constructed and a nonlinear control law derived that renders the manifold invariant, such that the restriction of the system dynamics on the invariant manifold represents the desirable target dynamics of the controlled system.
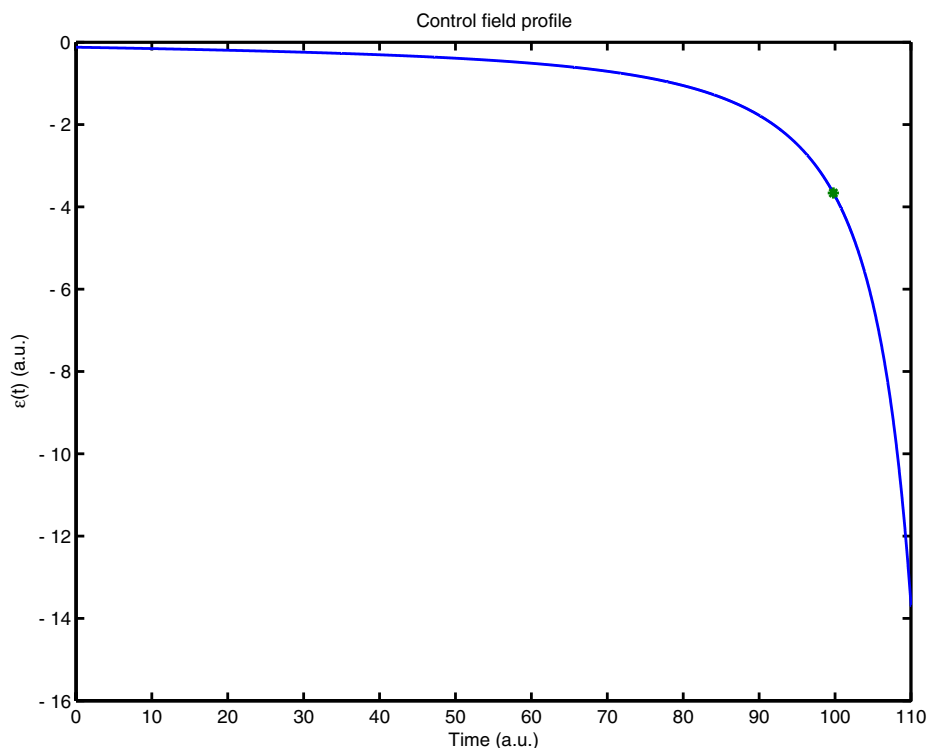
FIG. 2. *Control field profile.*

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