Slow Attractive Canonical Invariant Manifolds for Hydrogen-Air Kinetics

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***Abstract*— We illustrate the construction of a Slow Attractive Canonical Invariant Manifold (SACIM) by connection of equilibria by heteroclinic orbits for a model system of hydrogen-air kinetics. The SACIM is guaranteed invariant by virtue of its construction technique. For the case illustrated, a posteriori stretching- and rotation-based diagnostic methods show it is also slow and attractive. However, in that 1) manifolds so constructed need not be slow or attractive, and 2) no a priori method is yet available to construct a SACIM, the utility of the construction technique may be limited.**

I. Introduction

We highlight here some of our recent results that are more fully described in [1]. Spatially homogeneous chemical reactions are described by dynamical systems of the form

$$\frac{d\mathbf{z}}{dt} = \mathbf{f}(\mathbf{z}), \qquad \mathbf{z}(0) = \mathbf{z}_o, \qquad \mathbf{z}, \mathbf{z}_o, \mathbf{f} \in \mathbb{R}^N. \quad (1)$$

Here, $\mathbf{z}$ is a vector of length N containing the species concentrations, assuming that linear constraints representing element conservation have been removed, t is time, and $\mathbf{f}$ is a non-linear function of $\mathbf{z}$ representing the law of mass action with Arrhenius kinetics.

We take a Slow Attractive Canonical Invariant Manifold (SACIM) to be an invariant manifold (IM) on which slow dynamics are confined and to which nearby trajectories are attracted. We identify an IM to be a CIM when it is a heteroclinic connection of equilibria. The potential identification of one-dimensional SACIMs by CIM construction has gained attention since its introduction [2] and extension by others, *e.g.* [3], [4], [5]. The essence of the fundamental hypothesis is illustrated in Fig. 1. That hypothesis is that SACIMs may be constructed by 1) identifying equilibria of Eq. (1), *i.e.* points $\mathbf{z}$ where $\mathbf{f}(\mathbf{z}) = \mathbf{0}$, and 2) connecting by trajectories from appropriate non-physical saddle equilibria (those with at most one positive eigenvalue) to the unique physical equilibrium, which is a sink. Near the equilibria, the CIM is guaranteed to be attractive; moreover, for many reactive systems the CIM appears to be attractive in regions far from equilibrium.

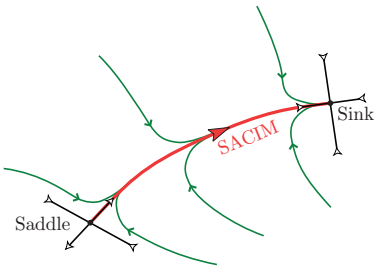

Fig. 1. Sketch of SACIM envisioned as the invariant manifold connecting equilibria.

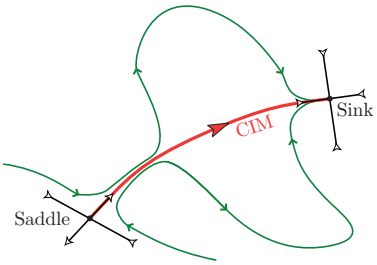

Fig. 2. Sketch of failure of the method of heteroclinic orbit construction for SACIM identifcation.

However, nothing in the construction algorithm precludes the scenario sketched in Fig. 2. Certainly, equilibria can be identified and connected via heteroclinic orbits to construct a CIM. But for a generic $\mathbf{f}(\mathbf{z})$, one has no guarantee that trajectories near the CIM are in fact attracted to it. In this study, we summarize the method and discuss an example given by Powers, *et al.* [1] for the model hydrogen-air problem introduced by Ren, *et al.* [6]. Our example will demonstrate a SACIM, while [1] gives another example where the method fails.

II. Summary of analysis

With the local Jacobian $\mathbf{J} = \partial\mathbf{f}/\partial\mathbf{z}$, defined throughout the entire phase space, one can analyze $\mathbf{J}$ in the neighborhood of any IM, such as a CIM connecting equilibria. At the physical equilibrium, all of the eigenvalues of $\mathbf{J}$ are guaranteed to be negative and real, and all nearby points will be drawn to the physical equilibrium. Away from the physical equilibrium, it is possible for some eigenvalues to be positive, and this can lead to certain trajectories being drawn away from a CIM. It is well known that $\mathrm{tr}\,(\mathbf{J})$ is proportional to the rate of change of a local volume in phase space. However, even if $\mathrm{tr}\,(\mathbf{J}) < 0$, the existence of a positive eigenvalue can induce a local repulsion of an individual trajectory from a CIM.

It is possible, see [1], [3], to identify a unit tangent vector to the CIM, $\boldsymbol{\alpha}_t$, and a set of unit normal vectors, $\boldsymbol{\alpha}_{n,i}, i = 1, \ldots, N-1$. These vectors can be used to identify the tangential and normal stretching rates, σ_t and $\sigma_{n,i}$:

$$\sigma_t = \boldsymbol{\alpha}_t^T \cdot \mathbf{J}_s \cdot \boldsymbol{\alpha}_t, \ \sigma_{n,i} = \boldsymbol{\alpha}_{n,i}^T \cdot \mathbf{J}_s \cdot \boldsymbol{\alpha}_{n,i}, \ i = 1, \ldots, N-1. \tag{2}$$

Here $\mathbf{J}_s = (\mathbf{J} + \mathbf{J}^T)/2$ is the symmetric part of $\mathbf{J}$. Along the CIM, $\boldsymbol{\alpha}_t$ is uniquely defined, up to its sign. However, there are an infinite set of $\boldsymbol{\alpha}_{n,i}$ when $N > 2$. Certainly if all possible $\sigma_{n,i} < 0$ and $\min_i |\sigma_{n,i}| \gg |\sigma_t|$, the CIM will be a SACIM; however, it is easy to construct cases for which these criteria are not met.

We can better understand the dynamics normal to the CIM by constructing

$$\mathbf{Q}_n = \begin{bmatrix} | & & | \\ \boldsymbol{\alpha}_{n,1} & \cdots & \boldsymbol{\alpha}_{n,N-1} \\ | & & | \end{bmatrix}, \tag{3}$$

where $\mathbf{Q}_n$ is an $N \times (N-1)$ rectangular matrix with orthonormal columns. Then, the normal Jacobian, $\mathbf{J}_n$ is found by projecting $\mathbf{J}$ onto this basis:

$$\mathbf{J}_n = \mathbf{Q}_n^T \cdot \mathbf{J} \cdot \mathbf{Q}_n. \tag{4}$$

As shown in [1], the eigenvalues/eigenvectors associated with the symmetric part of $\mathbf{J}_n$ describe the stretching dynamics; for $N = 3$, rotation dynamics are associated with the anti-symmetric part of $\mathbf{J}_n$.

III. Hydrogen-Air Example

We apply our method to a simple hydrogen-air combustion model [5], [6]. This model considers the six species H_2, O, H_2O, H, OH, and N_2. The six evolution equations for each species are reduced by elemental constraints to a system of $N = 3$ ordinary differential equations. We take then as dependent variables, z_1, z_2, and z_3, the specific moles of H_2, O, and H_2O. Algebraic analysis reveals seven finite equilibria that we label R_i, $i = 1, \ldots, 7$. The equilibrium R_7 is the unique physical equilibrium, and we can construct a CIM by connecting R_7 to R_1 and R_6. Stretching-based diagnostics reveal that on the path $R_1 \rightarrow R_7$, one of the extremal normal stretching rates is positive, for which the CIM could then be repulsive. This local repulsion is overcome however by fast local rotation of trajectories into regions of attraction. Figure 3 shows the SACIM for this system, and Fig. 4 shows how the local rotation of individual trajectories allows the CIM to be a SACIM.

IV. Conclusion

Construction of canonical invariant manifolds via connection of equilibria by heteroclinic orbits is possible for model hydrogen-air systems; it is possible to diagnose a posteriori if such manifolds are slow and attractive, but one has no a priori guarantee that manifolds so constructed are slow and attractive.

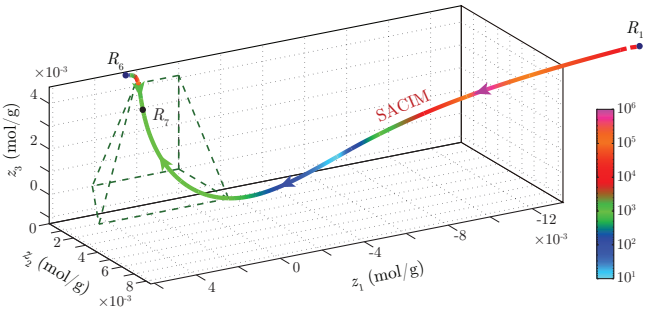

Fig. 3. The SACIMs for the simple hydrogen-air system are colored based on the relative slowness. The solid dots are finite critical points; R_7 represents the system's physical equilibrium state, R_1 and R_6 represent the starting points of the SACIMs, and the dashed simplex represents the physical domain.

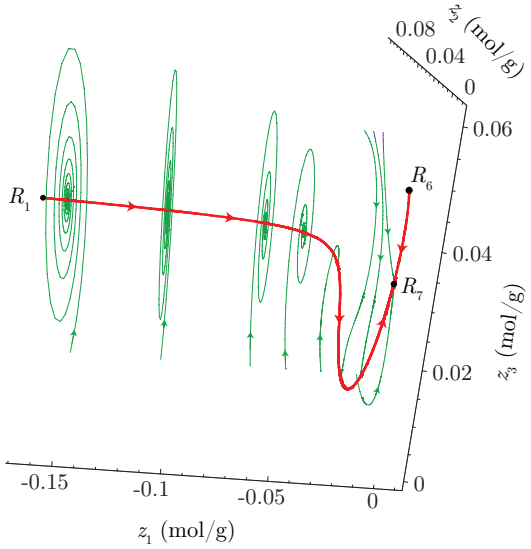

Fig. 4. Illustration exhibiting how the SACIMs for the simple hydrogen-air system attract nearby trajectories for both $R_1 \rightarrow R_7$ and $R_6 \rightarrow R_7$.

References

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