Challenges of Reduction for Open Systems

Joseph M. Powers*, Joshua D. Mengers†
*University of Notre Dame, Department of Aerospace and Mechanical Engineering, Notre Dame, Indiana, USA
†US Department of Energy, Geothermal Technologies Office, Washington, DC, USA

***Abstract*— Open spatially homogeneous reactive systems may possess multiple physical equilibria and display limit cycle behavior. It is demonstrated for two systems, i) a simple Gray-Scott model, and ii) a detailed hydrogen-air model, that the existence of multiple physical equilibria and limit cycles introduces challenges for the use of manifold methods as a reduction technique. In particular, detailed understanding of boundaries of basins of attraction is likely required in order for any reduction to maintain fidelity to the full model.**

I. Introduction

It is well known that open spatially homogeneous reactive systems may possess multiple physical equilbria and exhibit limit cycle behavior. Any stable physical equilbria, as well as any stable limit cycle, will also possess a basin of attraction, whose boundaries are difficult to discern without fully exploring a multi-dimensional phase space. It is also the case that many reduction methods rely upon projecting an arbitrary point in phase space onto a lower dimension manifold. One common method for identifying such manifolds which are one-dimensional is to connect equilbria with heteroclinic orbits and examine their ability to attract nearby orbits via calculation of normal stretching rates [1]. Those that are attractive are known as Slow Invariant Manifolds (SIMs). However, it must be recognized that naïve projection, uninformed by knowledge of the basins of attraction, from an arbitrary point onto a lower dimensional manifold runs the risk of projecting onto the wrong manifold. For cases in which there are multiple candidate SIMs, even less is clear, including how to define a basin of attraction for a SIM.

In this study, we summarize two such cases whose full exposition, including literature review, model equations, and numerical parameter values, is given by Mengers [2]. Those two cases are i) a simple Gray-Scott model, widely used to study pattern formation dynamics, and ii) a detailed kinetics model for hydrogen-air combustion.

II. Gray-Scott

The Gray-Scott model has two irreversible reactions in three species, U, V, and P: $U + 2V \rightarrow 3V$, $V \rightarrow P$. The spatially homogenous version is

$$\frac{dY_U}{dt} = -Y_U Y_V^2 + \mathsf{F}(1 - Y_U), \tag{1}$$

$$\frac{dY_V}{dt} = Y_U Y_V^2 - (\mathsf{F} + \mathsf{k}) Y_V. \tag{2}$$

Here Y represents mass fraction, t time, with $\mathsf{F} > 0$ and $\mathsf{k} > 0$ as parameters. One real finite root, $R_1 : (Y_U, Y_V) = (1, 0)$, is guaranteed to be a sink. The character of the other two roots depends on F and k. When $\mathsf{F} = 0.16 \times 10^{-3}$ and $\mathsf{k} = 3.1 \times 10^{-2}$, three real positive finite roots, R_1, R_2, and R_3, are found, plotted in Fig. 1a.

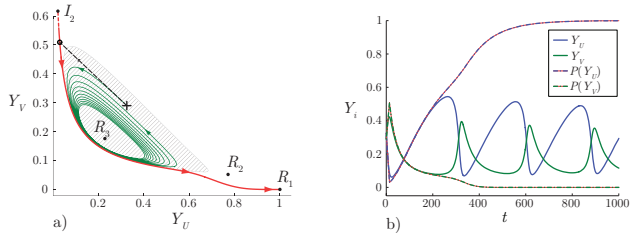

Fig. 1. Naïve projection onto a reduced manifold in the Gray-Scott system

The sink at R_1 has heteroclinic connections with the saddle at R_2 as well as the point at infinity at I_2. There is also a spiral source at R_3. Surrounding R_3 is an invariant manifold comprising a stable limit cycle, whose basin of attraction is shaded. Figure 1a depicts an initial condition within the basin of attraction of the limit cycle, denoted with a "+." Many reduction algorithms would project this point onto the manifold emanating from I_2, which leads ultimately to R_1. This induces large error, as the actual trajectory is led to the limit cycle surrounding R_3. Figure 1b depicts the evolution of Y_U and Y_V from "+" for its actual limit cycle behavior and that obtained upon naïve projection to the wrong reduced manifold.

III. Hydrogen-Air

We next employ a 9 species, 20 reaction hydrogen-air mechanism with a species ordering of $\{O_2, H_2, H_2O, N_2, OH, H, O, HO_2, H_2O_2\}$ in an isothermal, isochoric simulation of combustion with fresh mixture inflow balanced by exhaust. The system has 3 algebraic constraints; therefore, we can confine attention to species $i = \{1, 2, 3, 5, 6, 7\}$. We identify 97 real finite equilibria. Of these, 3 have positive concentrations for all 9 species, making them physical, and 13 have one positive eigenvalue, making them candidates for connection to the physical roots. For the physical equilibria, R_4 has all negative real eigenvalues and thus is a sink; R_{69} has one positive real eigenvalue, making it a candidate for connecting to other equlibria; and R_1 has four

negative real eigenvalues and one complex conjugate pair of eigenvalues with positive real part, making it a saddle. The long time dynamics of systems with initial conditions in the neighborhood of R_1 exhibit limit cycle behavior.

We integrate with initial conditions perturbed along R_{69}'s unstable eigenvector in either direction. In one direction, the trajectory approaches R_4 along its slowest eigenvector; this is a branch of the SIM. In the other direction, the trajectory collapses onto the limit cycle. These trajectories are shown in a projection of phase space in Fig. 2. Here z_i is the specific mole number of species i.

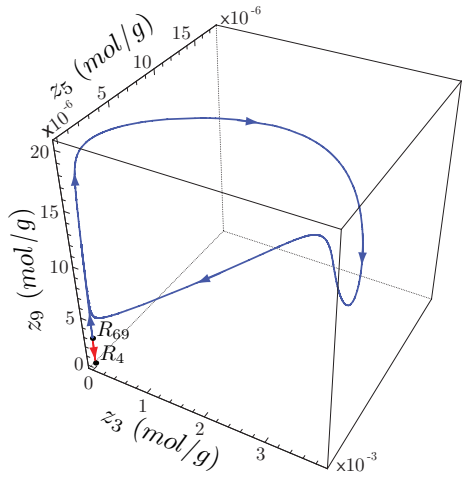

Fig. 2. The limit cycle and a SIM branch in the hydrogen-air mechanism.

Two time evolutions are shown in Fig. 3, where from nearly identical initial conditions, the top and bottom display relaxation to R_4 and the stable limit cycle, respectively. Thus, R_{69} lies on the boundary of the basin of attraction between the limit cycle and R_4. We can identify other branches of the SIM by examining the heteroclinic orbits from other candidate equilibria. We find four additional branches, emanating from R_9, R_{17}, R_{30}, and R_{53}, respectively. A projection of these branches' approach to the physical equilibrium sink, R_4, is shown in Fig. 4. To evaluate the attractiveness of these branches, we calculate the normal stretching ratio along each manifold. We find that all five normal stretching ratios remain negative along the entire length of both the R_{69} and R_{53} branches. Thus, both are candidates for a SIM, rendering it also useful to construct a basin of attraction for each, not done here. We find there are positive stretching ratios in multiple normal directions for a large portion of the branches near R_9, R_{17}, and R_{30}. This indicates nearby trajectories may diverge, an undesirable trait for a reduction.

IV. Conclusion

These results raise concerns about the heteroclinic orbit SIM construction technique for open systems in the absence

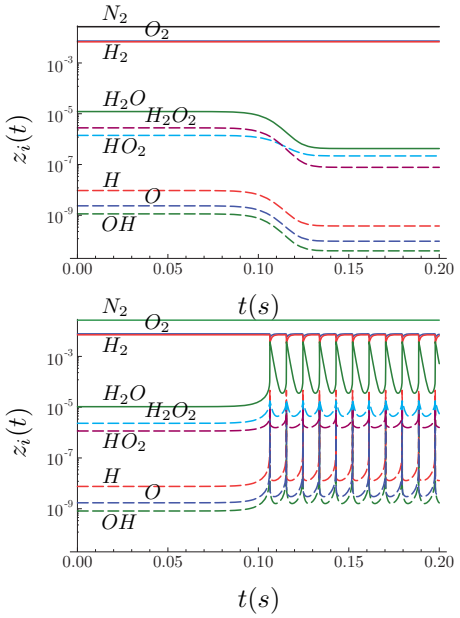

Fig. 3. Evolutions of hydrogen-air system from near R_{69}.

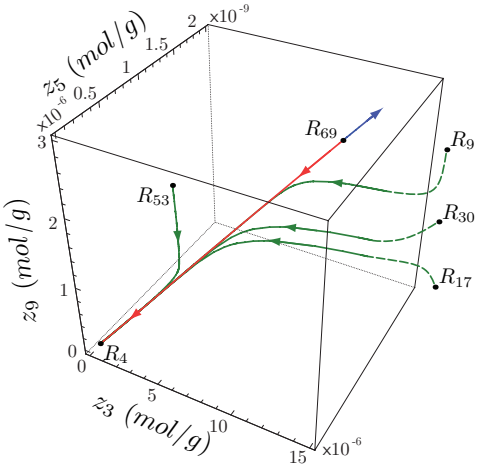

Fig. 4. Multiple branches of the SIM in the hydrogen-air mechanism.

of knowledge about the basins of attraction, which are difficult to obtain in practice.

Acknowledgments

The study was originally supported by the National Science Foundation under Grant No. CBET-0650843; partial support was also received in the form of a fellowship from the University of Notre Dame's Department of Applied and Computational Mathematics and Statistics.

References

[1] A. Adrover, F. Creta, M. Giona, and M. Valorani, "Stretching-based diagnostics and reduction of chemical kinetic models with diffusion," *Journal of Computational Physics* 225(2): 1442-1471.

[2] J. D. Mengers, 2012, "Slow invariant manifolds for reaction-diffusion systems," Ph.D. dissertation, University of Notre Dame.