Reduced Manifolds and Trajectory Curvature

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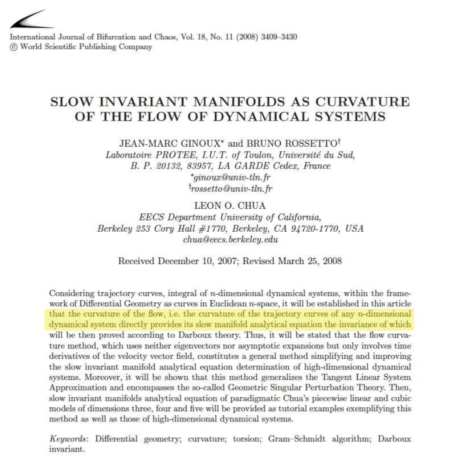
Taxonomy

We consider *Reduced Manifolds* for realistic spatially homogeneous gas phase kinetic systems.

- *Invariant Manifolds* (IMs) are sets of points which are invariant under the action of an underlying dynamic system.
- Any trajectory of a dynamic system is an IM.
- IMs may be locally or globally fast or slow, attracting or repelling.
- Slow or fast does not imply attracting or repelling and *vice versa*.
- The fast/slow and attracting/repelling nature of *Canonical Invariant Manifolds* (CIMs) constructed by connecting equilibria to determine *heteroclinic orbits* has been discussed by Powers, Paolucci, Mengers, Al-Khateeb, *J. Math. Chem.*, 2015.
- A global *Slow Attracting Canonical Invariant Manifold* (SACIM) may represent the *optimal reduction* potentially for enabling enhanced accuracy and efficiency in multiscale problems.

On the construction of SIMs

- It is relatively easy to construct CIMs by numerical integration.
- Many CIMs exist, but we are only interested in those that connect to physical equilibrium.
- It is desirable to identify those CIMs to which
  - dynamics are restricted to those which are *slow*, and
  - neighboring trajectories are rapidly *attracted*.
- Identification of these SACIMs is difficult.
- It is common in the literature to focus on *Slow Invariant Manifolds* (SIMs).
- As such, we will focus from hereon on SIMs, though we recognize a SACIM is more desirable.



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SLOW INVARIANT MANIFOLDS AS CURVATURE OF THE FLOW OF DYNAMICAL SYSTEMS

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Considering trajectory curves, integral of n-dimensional dynamical systems, within the framework of Differential Geometry as curves in Euclidean n-space, it will be established in this article that the curvature of the flow, i.e. the curvature of the trajectory curves of any n-dimensional dynamical system directly provides its slow manifold analytical equation the invariance of which will be then proved according to Darboux theory. Thus, it will be stated that the flow curvature method, which uses neither eigenvectors nor asymptotic expansions but only involves time derivatives of the velocity vector field, constitutes a general method simplifying and improving the slow invariant manifold analytical equation determination of high-dimensional dynamical systems. Moreover, it will be shown that this method generalizes the Tangent Linear System Approximation and encompasses the so-called Geometric Singular Perturbation Theory. Then, slow invariant manifolds analytical equation of paradigmatic Chua's piecewise linear and cubic models of dimensions three, four and five will be provided as tutorial examples exemplifying this method as well as those of high-dimensional dynamical systems.

Keywords: Differential geometry; curvature; torsion; Gram–Schmidt algorithm; Darboux invariant.

Ginoux, et al. have proposed an appealing SIM construction method based on differential geometry concepts such as local curvature and torsion of trajectories to identify SIMs.

- *Int. J. Bifurcation Chaos*, 2006, 2008
- *Qual. Theory Dyn. Syst.*, 2013, 2014

We will consider this method and compare its results to other methods.

Theoretical framework for spatially homogeneous combustion within a closed volume

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

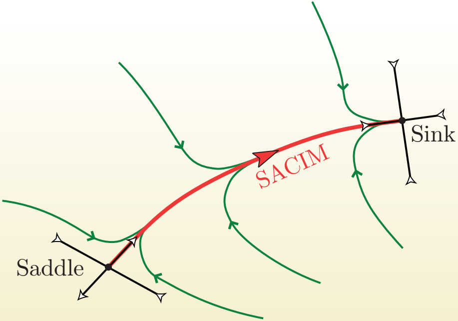
- $\mathbf{x}$, a *position* in phase space, represents a set of N specific mole numbers, assuming all linear constraints have been removed.
- $\mathbf{v}(\mathbf{x})$, a *velocity* in phase space, embodies the law of mass action.
- $\mathbf{v}(\mathbf{x}) = \mathbf{0}$ defines *multiple equilibria* within $\mathbb{R}^N$.
- $\mathbf{v}(\mathbf{x})$ is such that a *unique stable equilibrium* exists for physically realizable values of $\mathbf{x}$; the eigenvalues of the Jacobian

$$\mathbf{J} = \frac{\partial \mathbf{v}}{\partial \mathbf{z}},$$

  are guaranteed real and negative at such an equilibrium.
- $\mathbf{a}(\mathbf{x}) = \frac{\partial \mathbf{v}}{\partial \mathbf{x}} \frac{d\mathbf{x}}{dt} = \mathbf{J} \cdot \mathbf{v}$ is an *acceleration* in phase space.

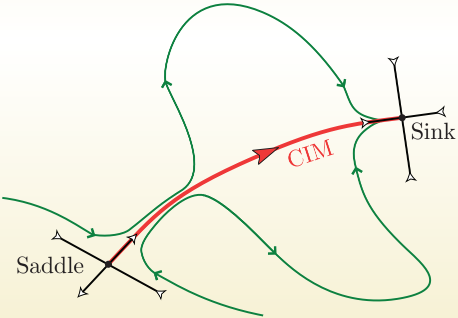
SACIM construction strategy: heteroclinic orbit connection

- Davis and Skodje suggested a CIM construction strategy.
- It employs numerical integration from a saddle to the sink.
- This guarantees a CIM.
- It *may* be a SACIM.

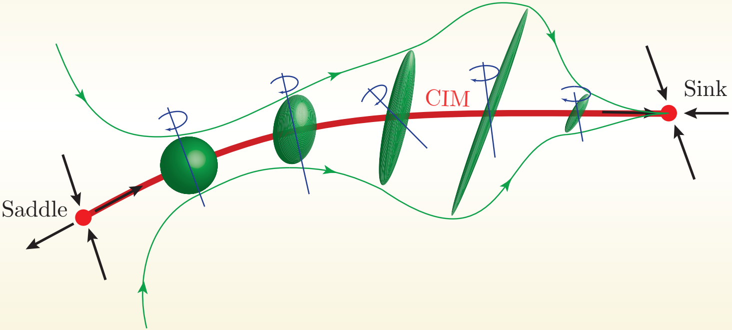


Failure of SACIM construction strategy

- It *may not* be a SACIM.
- The CIM will be attracting in the neighborhood of each equilibrium.
- The CIM need not be attractive away from either equilibrium.



Sketch of a volume locally traversing a nearby CIM



The local differential volume 1) translates, 2) stretches, and 3) rotates. Its magnitude can decrease as it travels, but elements can still be repelled from the CIM. All trajectories are ultimately attracted to the sink.

Based on rotation rate, one may determine whether or not the CIM is a SACIM; see Powers, et al. 2015.

Alternate SIM construction strategy of Ginoux, et al.

- Each trajectory possesses generalized curvature.
- For 2D trajectories, this is the ordinary curvature, κ:

$$\kappa = \frac{||\mathbf{a} \times \mathbf{v}||}{||\mathbf{v}||^3}$$

For 2D, Zero-Curvature Manifold (ZCM) when $\kappa = 0$.

- For 3D trajectories, one has the torsion τ:

$$\tau = -\frac{(\mathbf{v} \times \mathbf{a}) \cdot \frac{d\mathbf{a}}{dt}}{\kappa^2 ||\mathbf{v}||^6}$$

For 3D, ZCM when $\tau = 0$.

- In general, the ZCM is given by the condition

$$\det\left(\dot{\mathbf{x}}, \ddot{\mathbf{x}}, \ldots, \overset{(\mathrm{n})}{\mathbf{x}}\right) = 0.$$

- Claim: invariance of the ZCM established by the Darboux Theorem, provided $d\mathbf{J}/dt = \mathbf{0}$.

2D SIM construction strategy of Ginoux, et al.

- Trajectory curvature κ given by:

$$\kappa = \frac{||\mathbf{a} \times \mathbf{v}||}{||\mathbf{v}||^3}$$

- The ZCM is a set of points that have trajectories passing through it with velocity parallel to acceleration:

$$\text{ZCM}: \ \mathbf{a} \times \mathbf{v} = \mathbf{0}$$

- The ZCM is not a trajectory; trajectories passing through the ZCM possess zero curvature on the ZCM.
- The ZCM itself has non-zero curvature.
- It is claimed, Ginoux 2006, that the ZCM identifies the SIM.
- It is better stated that the ZCM approximates the SIM, and that the ZCM is not an IM.

A later cavaet from Ginoux, 2013

Note. Let's notice that the *slow invariant manifold* equation (9) associated with *n*-dimensional *singularly perturbed systems* defined by the *Flow Curvature Method* is a tensor of order *n*. As a consequence, it can only provide an approximation of *n*-order in ε of the *slow invariant manifold* equation (6). Nevertheless, it is easy to show that the Lie derivative of the "*slow manifold*" equation (9) obtained by the *Flow Curvature Method* can be written as:

$$L_{\vec{X}}\phi(\vec{X},\varepsilon) = \dot{\vec{X}} \cdot \left(\ddot{\vec{X}} \wedge \dddot{\vec{X}} \wedge \ldots \wedge \overset{(n+1)}{\vec{X}} \right) = \det\left(\dot{\vec{X}}, \ddot{\vec{X}}, \dddot{\vec{X}}, \ldots, \overset{(n+1)}{\vec{X}} \right) = 0 \quad (13)$$

This extension will not be analyzed here.

The Davis-Skodje system

A nonlinear system with similar properties to reaction-based systems:

$$\frac{dx}{dt} = -x, \qquad x(0) = x_0,$$
$$\frac{dy}{dt} = -\gamma y + \frac{(\gamma - 1)x + \gamma x^2}{(1+x)^2}, \qquad y(0) = y_0.$$

Exact solution:

$$x(t) = x_0 e^{-t},$$
$$y(t) = \frac{x_0 e^{-t}}{1 + x_0 e^{-t}} + \left(y_0 - \frac{x_0}{1 + x_0} \right) e^{-\gamma t}.$$

Exact solution in the phase plane:

$$y(x) = \frac{x}{1+x} + \left(y_0 - \frac{x_0}{1+x_0} \right) \left(\frac{x}{x_0} \right)^{\gamma}.$$

Davis-Skodje, cont.

For large stiffness, $\gamma \gg 1$, the SIM is approached from arbitrary initial conditions:

$$y_{SIM} = \frac{x}{1+x}.$$

Exact expressions exist for $\mathbf{J}$ and $\mathbf{a}$:

$$\mathbf{J} = \begin{pmatrix} -1 & 0 \\ \frac{\gamma-1+(\gamma+1)x}{(1+x)^3} & -\gamma \end{pmatrix},$$

$$\mathbf{a} = \begin{pmatrix} x \\ \gamma^2 y - \frac{x\left(\gamma^2(x+1)^2+x-1\right)}{(x+1)^3} \end{pmatrix}.$$

Eigenvalues of $\mathbf{J}$ are $\lambda_1 = -1$, $\lambda_2 = -\gamma$.

Davis-Skodje, cont.

$$\frac{d\mathbf{J}}{dt} = \begin{pmatrix} 0 & 0 \\ -\frac{2(\gamma+(\gamma+1)x-2)\dot{x}}{(x+1)^4} & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ \frac{2x(\gamma+\gamma x+x-2)}{(x+1)^4} & 0 \end{pmatrix} \neq \mathbf{0}.$$

The condition for the Darboux Theorem required for an IM is not met. So there is no guarantee that a ZCM is an IM.

ILDM for the Davis-Skodje system

The Maas-Pope Intrinsic Low-Dimensional Manifold (ILDM) is found by projecting the system onto a basis from fast and slow modes of **J** and equilibrating the equation associated for the fast time scale. For the Davis-Skodje system, this yields the ILDM:

$$y_{ILDM} = \underbrace{\frac{x}{x+1}}_{y_{SIM}} + \frac{2x^2}{\gamma(\gamma-1)(1+x)^3}.$$

Obviously, y_{ILDM} is not a SIM, but approaches the SIM as $\gamma \to \infty$.

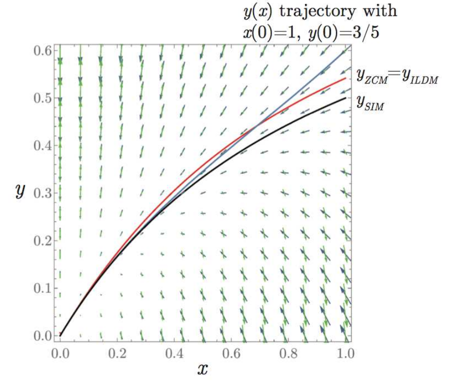
ZCM for the Davis-Skodje system

The ZCM is found by enforcing $\mathbf{a} \times \mathbf{v} = \mathbf{0}$. For the Davis-Skodje system, this yields the ZCM:

$$y_{ZCM} = \underbrace{\frac{x}{x+1}}_{y_{SIM}} + \frac{2x^2}{\gamma(\gamma-1)(1+x)^3}.$$

For the Davis-Skodje system, the ZCM is the ILDM, and is not the SIM. The ZCM is not a solution trajectory, and it is not an IM. As does the ILDM, the ZCM approaches the SIM as $\gamma \to \infty$.

Davis-Skodje system for $\gamma = 3$



- Consider $x = 1$.
- Here $dx/dt = -1$, $dy/dt = -1/4$, so $dy/dx = 1/4$.
- Direct differentiation of the SIM gives $dy_{SIM}/dx|_{x=1} = 1/4$.
- Here $y_{ZCM} = 13/24$, and on the ZCM at $x = 1$, $dy/dx = 3/8$
- But at $x = 1$, $dy_{ZCM}/dx|_{x=1} = 13/48$.

Conclusions

- The ZCM has non-zero curvature.
- Trajectories that pass through the ZCM do so with their velocity parallel to their acceleration, thus rendering the trajectories to have no curvature at the ZCM.
- The ZCM is an ILDM.
- The ZCM is not a SIM.
- The ZCM and ILDM better approximate the SIM as stiffness increases.
- Later extensions to the theory of ZCMs remain to be analyzed for the Davis-Skodje system.

Conclusions

As shown elsewhere,

- A SACIM represents a “gold standard” for a reduced kinetics model for a spatially homogeneous reactive system.
- SACIMs can be identified in physically-based gas phase kinetics systems.
- SACIM diagnosis is arduous for small systems, unclear for systems of higher dimension than three, and presently impractical for engineering combustion applications.

Relevant to the discussion here,

- ZCMs for large practical systems of realistic kinetics have not yet been identified.
- Such a task is likely arduous as well.