The slowness of invariant manifolds constructed by connection of heteroclinic orbits

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Some motivating questions...

We wish to use manifold methods to filter and reduce challenging multi-scale problems, but such methods are burdened with many questions:

- Just what is a *SACIM*?:
  - Slow,
  - Attracting,
  - Canonical,
  - Invariant,
  - Manifold.
- Does it exist?
- Is it easy to identify?
- Does it actually work?
On the Existence of a Slow Manifold

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ABSTRACT

We identify the slow manifold of a primitive-equation system with the set of all solutions that are completely devoid of gravity-wave activity. We construct a five-variable model describing coupled Rossby waves and gravity waves. Successive-approximation schemes designed to determine the slow manifold fail to converge when applied to the model, although they sometimes appear to converge before finally diverging. A noniterative scheme which demands only that the fast variables be functions of the slow variables yields a “slowest invariant manifold,” which, however, is not unequivocally slow. We question whether the complete absence of gravity waves can be logically defined, and we note that the existence or nonexistence of a slow manifold does not depend upon the convergence or nonconvergence of a power series or a succession of approximations.

(focused on the related topic of limit cycles)
On the Nonexistence of a Slow Manifold

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ABSTRACT

We define the slow manifold $S$ in the state space of a primitive-equation model as a hypothetical invariant manifold on which there is no gravity-wave activity, and on which unique velocity-potential and streamfunction fields correspond to each isobaric-height field. We introduce a five-variable forced damped model, and show that for this model the point $H$ representing the Hadley circulation and the two orbits forming the unstable manifold of $H$ must lie in $S$ if $S$ exists. We then show that in traveling along one of these orbits one eventually encounters gravity waves, whereupon it follows that $S$ does not exist.

A measure $G$ of gravity-wave activity is found to decrease very rapidly as the external forcing $F$ decreases. An approximate formula is derived for $G$ as a function of $F$.

We show that a particular nine-variable forced damped model with orography also fails to possess a slow manifold, and we speculate as to the existence of slow manifolds in larger and more realistic models.
and for which questions remain!

2450

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The Slow Manifold—What Is It?

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ABSTRACT

Two studies that disagree as to whether a slow manifold is present in a particular low-order primitive equation model are compared. It is shown that the discrepancy occurs because of a difference of opinion as to what constitutes a slow manifold.
\textbf{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 \textit{vice versa}.

We will evaluate the fast/slow and attracting/repelling nature of \textit{Canonical Invariant Manifolds} (CIMs) constructed by connecting equilibria to determine \textit{heteroclinic orbits} (Davis-Skodje, 1999).
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.

We call such CIMs *Slow Attracting Canonical Invariant Manifolds* (SACIMs).

A global SACIM may represent the *optimal reduction* potentially enabling dramatic computational accuracy and efficiency in multiscale problems.

Manifolds identified by Davis-Skodje construction are guaranteed to be CIMs; they are not guaranteed to be SACIMs, even locally!
We analyze by expanding on the stretching-based diagnostic tools, in the limit of zero diffusion, described by


For discussion of the impact of diffusion on SACIMs, see

Theoretical framework for spatially homogeneous combustion within a closed volume

\[ \frac{dz}{dt} = f(z), \quad z(0) = z_0, \quad z, z_0, f \in \mathbb{R}^N. \]

- \( z \) represents a set of \( N \) species concentrations, assuming all linear constraints have been removed.
- \( f(z) \) embodies the law of mass action and other thermochemistry.
- \( f(z) = 0 \) defines multiple equilibria within \( \mathbb{R}^N \).
- \( f(z) \) is such that a unique stable equilibrium exists for physically realizable values of \( z \); the eigenvalues of the Jacobian

\[ J = \frac{\partial f}{\partial z}, \]

are guaranteed real and negative at such an equilibrium (Powers & Paolucci, *American Journal of Physics*, 2008).
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.
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.
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.
Local decomposition of motion

\[
\frac{dz}{dt} = f(z), \quad z(0) = z_o, \quad z_o \in \text{CIM},
\]

\[
\frac{d}{dt}(z - z_o) = f(z_o) + J_s|_{z_o} \cdot (z - z_o) + J_a|_{z_o} \cdot (z - z_o) + \ldots.
\]

Here, we have

\[
J = \frac{\partial f}{\partial z} = J_s + J_a,
\]

\[
J_s = \frac{J + J^T}{2}, \quad J_a = \frac{J - J^T}{2}.
\]

The symmetry of \(J_s\) allows definition of a real orthonormal basis.

In 3d, the rotation vector \(\omega\) of the anti-symmetric \(J_a\) defines the axis of rotation; can be extended for higher dimensions.
The local relative volumetric stretching rate is

\[
\frac{1}{V} \frac{dV}{dt} \equiv \ln V = \text{tr}J = \text{tr}J_s.
\]

The stretching rate \(\sigma\) associated with any unit vector \(\alpha\) is

\[
\sigma = \alpha^T \cdot J \cdot \alpha = \alpha^T \cdot J_s \cdot \alpha.
\]

The above result is general; \(\alpha\) need not be an eigenvector of \(J\) or \(J_s\), and \(\sigma\) need not be an eigenvalue of \(J\) or \(J_s\).

If they were eigenvalue/eigenvector pairs of \(J_s\), they would represent the principal axes of stretch and the associated principal values.
Consider now the motion along a given CIM:

- The unit tangent vector, $\alpha_t$, need not be a principal axis of stretch.
- The tangential stretching rate, $\sigma_t = \alpha_t^T \cdot J_s \cdot \alpha_t$, can be positive or negative.
- The normal stretching rates, $\sigma_{n,i} = \alpha_{n,i}^T \cdot J_s \cdot \alpha_{n,i}$, can be positive or negative.
- The sum of stretching rates equals the relative volumetric stretching rate:

$$\dot{\ln V} = \text{tr}J = \text{tr}J_s = \sigma_t + \sigma_{n,1} + \cdots + \sigma_{n,N-1}.$$
Necessary conditions for a SACIM

- For a *slow* CIM, attraction *to* the CIM must be faster than motion *on* the CIM (a type of *normal hyperbolicity*):

  \[ \kappa \equiv \frac{\min_i |\sigma_{n,i}|}{|\sigma_t|} \gg 1. \]

- for an *attractive* CIM, either
  - *all* normal stretching rates, \(\sigma_{n,i}\), must be negative,

    \[ \sigma_{n,i} < 0, \quad i = 1, \ldots, N - 1, \]

  - or, if *some* of the normal stretching rates are positive, then
    - the relative volumetric stretching rate must be negative,

      \[ \dot{\ln} V < 0, \quad \text{and} \]

    - the local rotation rate must be much greater than the largest normal stretching rate,

      \[ \mu \equiv \frac{|\omega|}{\max_i \sigma_{n,i}} = \frac{||J_a||}{\max_i \sigma_{n,i}} \gg 1. \]
Procedure for local SACIM identification

- Identify all equilibria \( f(z) = 0 \).
- Determine the Jacobian, \( J = \partial f / \partial z \).
- Evaluate \( J \) near each equilibrium to determine its source, sink, saddle, etc. character.
- Numerically integrate from candidate saddles into the unique physical sink to determine a CIM, \( z_{CIM} \), which is a candidate SACIM.
- Numerically determine the unit tangent, \( \alpha_t \), along the CIM:
  \[
  \alpha_t = \frac{f(z_{CIM})}{||f(z_{CIM})||}.
  \]
- Determine the tangential stretching rate, \( \sigma_t \), via
  \[
  \sigma_t = \alpha_t^T \cdot J_s \cdot \alpha_t = \alpha_t^T \cdot J \cdot \alpha_t.
  \]
Use a Gram-Schmidt procedure to identify $N - 1$ unit normal vectors, thus forming the orthonormal basis

$$\{\alpha_t, \alpha_{n,1}, \ldots, \alpha_{n,N-1}\}.$$

Note that $\alpha_{n,i}$ are not eigen-directions of $J$, so the procedure works for non-normal systems, though questions remain for highly non-normal, near singular systems.

Form the $N \times (N - 1)$ orthogonal matrix $Q_n$ composed of the unit normal vectors

$$Q_n = \begin{pmatrix}
\vdots & \vdots & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
\alpha_{n,1} & \alpha_{n,2} & \cdots & \alpha_{n,N-1} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots
\end{pmatrix}.$$
Procedure for local SACIM identification, conc.

- Form the reduced $(N - 1) \times (N - 1)$ Jacobian $J_n$ for the motion in the hyperplane normal to the CIM:

  $$J_n = Q_n^T \cdot J_s \cdot Q_n.$$  

- Find the eigenvalues and eigenvectors of $J_n$. The eigenvalues give the extreme values of normal stretching rates $\sigma_{n,i}, i = 1, \ldots, N - 1$. The normalized eigenvectors of $J_n$ give the directions associated with the extreme values of normal stretching, $\alpha_{n,i}$.

- We have thus

  $$\sigma_{n,i} = \alpha_{n,i}^T \cdot J \cdot \alpha_{n,i} = \alpha_{n,i}^T \cdot J_s \cdot \alpha_{n,i}, \quad i = 1, \ldots, N - 1.$$  

- Identify $J_a$ and then $\omega$ and $|\omega|$. Note that $|\omega| = \sqrt{-\text{tr}(J_a \cdot J_a)/2}$. 

Example

- Model equations:

\[
\begin{align*}
\frac{dz_1}{dt} &= \frac{1}{20}(1 - z_1^2), \\
\frac{dz_2}{dt} &= -2z_2 - \frac{35}{16}z_3 + 2(1 - z_1^2)z_3, \\
\frac{dz_3}{dt} &= z_2 + z_3.
\end{align*}
\]

- Jacobian:

\[
J = \begin{pmatrix}
-\frac{z_1}{10} & 0 & 0 \\
-4z_1z_3 & -2 & -\frac{35}{16} + 2(1 - z_1^2) \\
0 & 1 & 1
\end{pmatrix}.
\]

- Two finite equilibria:
  - “non-physical” saddle at \( R_1 : (z_1, z_2, z_3)^T = (-1, 0, 0)^T \), and a
  - “physical” sink at \( R_2 : (z_1, z_2, z_3)^T = (1, 0, 0)^T \).
Relative volumetric deformation rate:

\[
\frac{1}{V} \frac{dV}{dt} = \dot{\ln V} = \text{tr} J = -1 - \frac{z_1}{10}.
\]

The CIM composed of the heteroclinic orbit connecting the saddle at $R_1$ to the sink at $R_2$ is the line

\[z_1 = s, \quad z_2 = 0, \quad z_3 = 0, \quad s \in [-1, 1].\]

For the *entire* CIM, the relative volume deformation rate is negative:

\[\dot{\ln V} \in \left[-\frac{11}{10}, -\frac{9}{10}\right].\]

By inspection, $\alpha_t = (1, 0, 0)^T$.

Thus, the tangential stretching rate is

\[\sigma_t = \alpha_t^T \cdot J \cdot \alpha_t = -\frac{z_1}{10},\]

which gives $\sigma_t \in [1/10, -1/10]$ on the CIM from $R_1$ to $R_2$. 
A trivial Gram-Schmidt procedure yields \( \alpha_{n,1} = (0, 1, 0)^T \) and \( \alpha_{n,2} = (0, 0, 1)^T \), and thus

\[
Q_n = \begin{pmatrix}
0 & 0 \\
1 & 0 \\
0 & 1
\end{pmatrix}.
\]

On the CIM,

\[
J = \begin{pmatrix}
-\frac{z_1}{10} & 0 & 0 \\
0 & -2 & -\frac{35}{16} + 2(1 - z_1^2) \\
0 & 1 & 1
\end{pmatrix},
\]

\[
J_s = \begin{pmatrix}
-\frac{z_1}{10} & 0 & 0 \\
0 & -2 & -\frac{19}{32} + 1 - z_1^2 \\
0 & -\frac{19}{32} + 1 - z_1^2 & 1
\end{pmatrix},
\]

and

\[
\omega = (-51/32 + 1 - z_1^2, 0, 0)^T, \quad |\omega| \sim 1.
\]
Example, cont.: $J_n$ and $\sigma_{n,i}$

- The reduced Jacobian for the normal hyperplane is
  \[
  J_n = Q_n^T \cdot J_s \cdot Q_n = \begin{pmatrix}
  -2 & -\frac{19}{32} + 1 - z_1^2 \\
  -\frac{19}{32} + 1 - z_1^2 & 1
  \end{pmatrix}.
  \]

- The eigenvalues of $J_n$ give $\sigma_{n,i}$:
  \[
  \sigma_{n,i} = -\frac{1}{2} \pm \frac{\sqrt{2473 - 832z_1^2 + 1024z_1^4}}{32}.
  \]

- $\sigma_{n,1} \sim 1$ for $z_1 \in [-1, 1]$; potential divergence from CIM.
- $\sigma_{n,2} \sim -2$ for $z_1 \in [-1, 1]$.
- $\kappa \sim 10$; thus, the CIM is slow.
- $|\omega| \sim \sigma_{n,1} \sim 1$; $\mu \sim 1$: the rotation is slow enough to allow some trajectories to diverge from the CIM away from equilibrium.
- Positive normal stretching does not guarantee divergence from the CIM; it permits it. Rotation can orient a volume into a region where trajectories diverge from the CIM. Near $R_1$, the time spent in convergent regions overwhelms that spent in divergent regions.
Example, cont.: CIM is not a SACIM!

- There are regions of the CIM which do not attract nearby trajectories in the region far from equilibrium.
- This reflects the local influence of a positive normal stretching rate, $\sigma_{n,1} \sim 1$ whose influence is realized due to modest local rotation, $|\omega| \sim 1$.
- Projection onto the CIM in regions away from equilibrium would thus induce significant error in the prediction of certain state variables.
The example shares important features with combustion systems:
- unique stable physical equilibrium, and
- non-physical saddle equilibrium.

The example may not share other important features with combustion systems:
- no obvious imposed constraints from conserved variables, and
- no clear entropy scalar guaranteed to be increasing on any physical path to equilibrium.

An upcoming example from Friday’s Powers/Mengers talk will explore relevant extensions to $H_2$/air combustion, along with open systems, multiple physical equilibria, and limit cycles.

We, with A. N. al-Khateeb, have stretching-based diagnostics.

Preliminary results indicate we have here a SACIM.
A question which extends beyond combustion!

Note: attraction also needed!
Conclusions and questions

- Lorenz asked and answered “The slow manifold—what is it?”
- The more fundamental question, “The slow manifold—where is it?,“ remains to be answered robustly.
- Stretching- and rotation-based diagnostics have utility in answering a related question, “When is a CIM a SACIM?”
- Our example showed for a problem with one universally positive normal stretching rate that local repulsion from a CIM was possible, overcome only near an equilibrium sink.
- Thus, heteroclinic orbit connection is not guaranteed to identify a SACIM.
- If the method of heteroclinic connection of equilibria cannot identify a SACIM, can any method do so?
- Our Friday talk will consider open systems, multiple equilibria, and limit cycles, and raise further fundamental questions!