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 multiscale 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?

These are old questions....

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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 which understanding has varied with time....

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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 JOURNAL OF THE ATMOSPHERIC SCIENCES VOL. 49, NO. 24

The Slow Manifold—What Is It?

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(Manuscript received 17 June 1991, in final form 17 March 1992)

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.

Taxonomy

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

Taxonomy, cont.

- 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!

Brief review

We analyze by expanding on the stretching-based diagnostic tools, in the limit of zero diffusion, described by

- Adrover, Creta, Giona, and Valorani, 2007, Stretching-based diagnostics and reduction of chemical kinetic models with diffusion, *Journal of Computational Physics*, 225(2): 1442-1471.
- Mengers, 2012, Slow invariant manifolds for reaction-diffusion systems, Ph.D. Dissertation, University of Notre Dame.

For discussion of the impact of diffusion on SACIMs, see

- Mengers and Powers, 2013, One-dimensional slow invariant manifolds for fully coupled reaction and micro-scale diffusion, *SIAM Journal on Applied Dynamical Systems*, 12(2): 560-595.

Theoretical framework for spatially homogeneous combustion within a closed volume

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

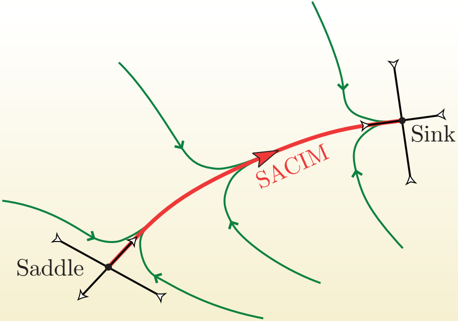
- $\mathbf{z}$ represents a set of N species concentrations, assuming all linear constraints have been removed.
- $\mathbf{f}(\mathbf{z})$ embodies the law of mass action and other thermochemistry.
- $\mathbf{f}(\mathbf{z}) = \mathbf{0}$ defines *multiple equilibria* within $\mathbb{R}^N$.
- $\mathbf{f}(\mathbf{z})$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

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

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

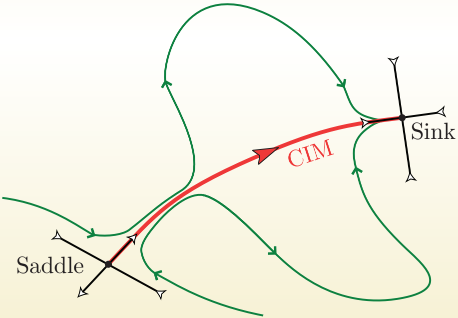
SACIM construction strategy: heteroclinic orbit connection

- 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.

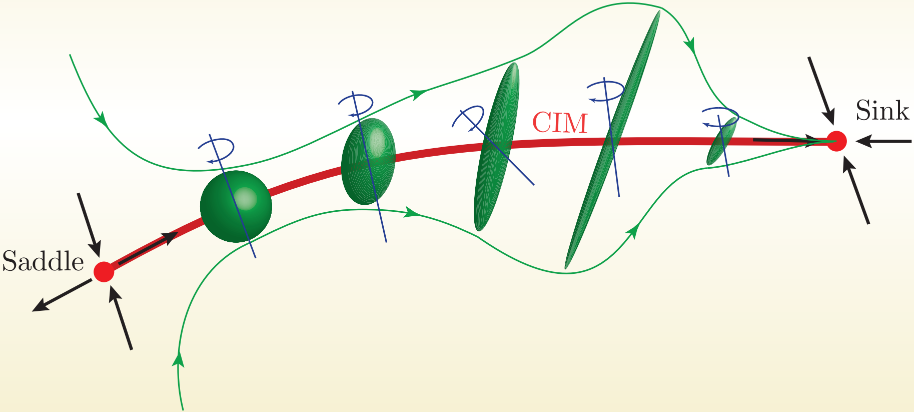


Failure of SACIM construction strategy

- 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.

Local decomposition of motion

$$\begin{aligned}\frac{d\mathbf{z}}{dt} &= \mathbf{f}(\mathbf{z}), \qquad \mathbf{z}(0) = \mathbf{z}_o, \qquad \mathbf{z}_o \in \text{CIM}, \\ \frac{d}{dt}(\mathbf{z} - \mathbf{z}_o) &= \underbrace{\mathbf{f}(\mathbf{z}_o)}_{\text{translation}} + \underbrace{\mathbf{J}_s\big|_{\mathbf{z}_o} \cdot (\mathbf{z} - \mathbf{z}_o)}_{\text{stretch}} + \underbrace{\mathbf{J}_a\big|_{\mathbf{z}_o} \cdot (\mathbf{z} - \mathbf{z}_o)}_{\text{rotation}} + \dots.\end{aligned}$$

Here, we have

$$\mathbf{J} = \frac{\partial \mathbf{f}}{\partial \mathbf{z}} = \mathbf{J}_s + \mathbf{J}_a,$$
$$\mathbf{J}_s = \frac{\mathbf{J} + \mathbf{J}^T}{2}, \quad \mathbf{J}_a = \frac{\mathbf{J} - \mathbf{J}^T}{2}.$$

The symmetry of $\mathbf{J}_s$ allows definition of a real orthonormal basis.

In 3d, the rotation vector $\boldsymbol{\omega}$ of the anti-symmetric $\mathbf{J}_a$ defines the axis of rotation; can be extended for higher dimensions.

Stretching rates

- The local relative volumetric stretching rate is

$$\frac{1}{V}\frac{dV}{dt} \equiv \dot{\overline{\ln V}} = \mathrm{tr}\mathbf{J} = \mathrm{tr}\mathbf{J}_s.$$

- The stretching rate σ associated with *any* unit vector $\boldsymbol{\alpha}$ is

$$\sigma = \boldsymbol{\alpha}^T \cdot \mathbf{J} \cdot \boldsymbol{\alpha} = \boldsymbol{\alpha}^T \cdot \mathbf{J}_s \cdot \boldsymbol{\alpha}.$$

- The above result is general; $\boldsymbol{\alpha}$ need not be an eigenvector of $\mathbf{J}$ or $\mathbf{J}_s$, and σ need not be an eigenvalue of $\mathbf{J}$ or $\mathbf{J}_s$.
- If they were eigenvalue/eigenvector pairs of $\mathbf{J}_s$, they would represent the principal axes of stretch and the associated principal values.

Stretching rates, cont.

Consider now the motion along a given CIM:

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

$$\dot{\overline{\ln V}} = \mathrm{tr}\mathbf{J} = \mathrm{tr}\mathbf{J}_s = \sigma_t + \sigma_{n,1} + \cdots + \sigma_{n,N-1}.$$

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,

$$\overline{\dot{\ln V}} < 0, \qquad \underline{\text{and}}$$

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

$$\mu \equiv \frac{|\boldsymbol{\omega}|}{\max_i \sigma_{n,i}} = \frac{||\mathbf{J}_a||}{\max_i \sigma_{n,i}} \gg 1.$$

Procedure for local SACIM identification

- Identify all equilibria $\mathbf{f}(\mathbf{z}) = \mathbf{0}$.
- Determine the Jacobian, $\mathbf{J} = \partial \mathbf{f} / \partial \mathbf{z}$.
- Evaluate $\mathbf{J}$ 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, $\mathbf{z}_{CIM}$, which is a candidate SACIM.
- Numerically determine the unit tangent, $\boldsymbol{\alpha}_t$, along the CIM:

$$\boldsymbol{\alpha}_t = \frac{\mathbf{f}(\mathbf{z}_{CIM})}{||\mathbf{f}(\mathbf{z}_{CIM})||}.$$

- Determine the tangential stretching rate, σ_t, via

$$\sigma_t = \boldsymbol{\alpha}_t^T \cdot \mathbf{J}_s \cdot \boldsymbol{\alpha}_t = \boldsymbol{\alpha}_t^T \cdot \mathbf{J} \cdot \boldsymbol{\alpha}_t.$$

Procedure for local SACIM identifcation, cont.

- Use a Gram-Schmidt procedure to identify $N-1$ unit normal vectors, thus forming the orthonormal basis

$$\left\{\boldsymbol{\alpha}_t, \boldsymbol{\alpha}_{n,1}, \ldots, \boldsymbol{\alpha}_{n,N-1}\right\}.$$

  Note that $\boldsymbol{\alpha}_{n,i}$ are not eigen-directions of $\mathbf{J}$, 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 $\mathbf{Q}_n$ composed of the unit normal vectors

$$\mathbf{Q}_n = \begin{pmatrix} \vdots & \vdots & \vdots & \vdots \\ \boldsymbol{\alpha}_{n,1} & \boldsymbol{\alpha}_{n,2} & \vdots & \boldsymbol{\alpha}_{n,N-1} \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix}.$$

Procedure for local SACIM identification, conc.

- Form the reduced $(N-1)\times(N-1)$ Jacobian $\mathbf{J}_n$ for the motion in the hyperplane normal to the CIM:

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

- Find the eigenvalues and eigenvectors of $\mathbf{J}_n$. The eigenvalues give the extreme values of normal stretching rates $\sigma_{n,i}$, $i = 1, \ldots, N-1$. The normalized eigenvectors of $\mathbf{J}_n$ give the directions associated with the extreme values of normal stretching, $\boldsymbol{\alpha}_{n,i}$.
- We have thus

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

- Identify $\mathbf{J}_a$ and then $\boldsymbol{\omega}$ and $|\boldsymbol{\omega}|$. Note that $|\boldsymbol{\omega}| = \sqrt{-\mathrm{tr}(\mathbf{J}_a \cdot \mathbf{J}_a)/2}$.

Example

- Model equations:

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

- Jacobian:

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

- 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 $R_2 : (z_1, z_2, z_3)^T = (1, 0, 0)^T$.

Example, cont.: dV/dt, IM, and σ_t

- Relative volumetric deformation rate:

$$\frac{1}{V}\frac{dV}{dt} = \dot{\overline{\ln V}} = \mathrm{tr}\mathbf{J} = -1 - \frac{z_1}{10}.$$

- 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:

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

- By inspection, $\boldsymbol{\alpha}_t = (1, 0, 0)^T$.
- Thus, the tangential stretching rate is

$$\sigma_t = \boldsymbol{\alpha}_t^T \cdot \mathbf{J} \cdot \boldsymbol{\alpha}_t = -\frac{z_1}{10},$$

which gives $\sigma_t \in [1/10, -1/10]$ on the CIM from R_1 to R_2.

Example, cont.: $\mathbf{Q}_n$, $\mathbf{J}$, and $\mathbf{J}_s$

- A trivial Gram-Schmidt procedure yields $\boldsymbol{\alpha}_{n,1} = (0,1,0)^T$ and $\boldsymbol{\alpha}_{n,2} = (0,0,1)^T$, and thus

$$\mathbf{Q}_n = \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

- On the CIM,
  - $$\mathbf{J} = \begin{pmatrix} -\frac{z_1}{10} & 0 & 0 \\ 0 & -2 & -\frac{35}{16} + 2(1 - z_1^2) \\ 0 & 1 & 1 \end{pmatrix},$$
  - $$\mathbf{J}_s = \begin{pmatrix} -\frac{z_1}{10} & 0 & 0 \\ 0 & -2 & -\frac{19}{32} + 1 - z_1^2 \\ 0 & -\frac{19}{32} + 1 - z_1^2 & 1 \end{pmatrix}, \qquad \text{and}$$
  - $\boldsymbol{\omega} = (-51/32 + 1 - z_1^2, 0, 0)^T$, $|\boldsymbol{\omega}| \sim 1$.

Example, cont.: $\mathbf{J}_n$ and $\sigma_{n,i}$

- The reduced Jacobian for the normal hyperplane is

$$\mathbf{J}_n = \mathbf{Q}_n^T \cdot \mathbf{J}_s \cdot \mathbf{Q}_n = \begin{pmatrix} -2 & -\frac{19}{32} + 1 - z_1^2 \\ -\frac{19}{32} + 1 - z_1^2 & 1 \end{pmatrix}.$$

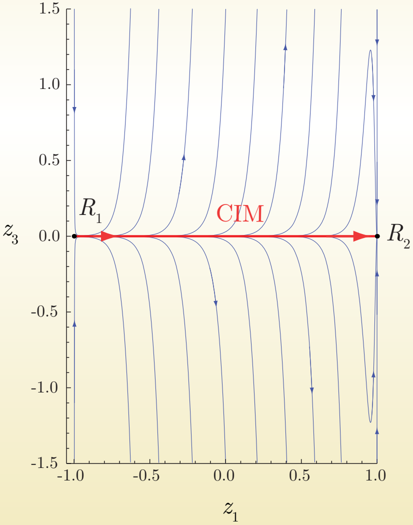
- The eigenvalues of $\mathbf{J}_n$ give $\sigma_{n,i}$:

$$\sigma_{n,i} = -\frac{1}{2} \pm \frac{\sqrt{2473 - 832 z_1^2 + 1024 z_1^4}}{32}.$$

- $\sigma_{n,1} \sim 1$ 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.
- $|\boldsymbol{\omega}| \sim \sigma_{n,1} \sim 1$; $\mu \sim 1$: 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!

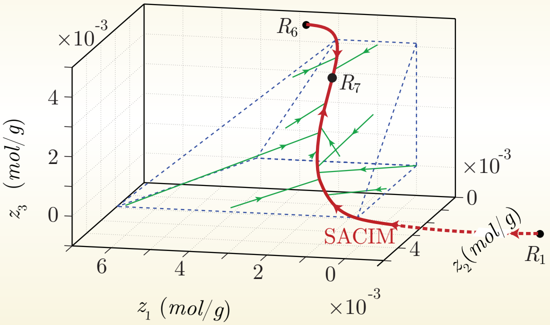
- There are regions of the CIM which do not attract nearby trajectories in the region far from equilibrium.
- This reflects the local influence of a positive normal stretching rate, $\sigma_{n,1} \sim 1$ whose influence is realized due to modest local rotation, $|\boldsymbol{\omega}| \sim 1$.
- Projection onto the CIM in regions away from equilibrium would thus induce significant error in the prediction of certain state variables.



Implications for combustion systems

- 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.

Preliminary results for H_2-air kinetics



- Six species model of Ren, Pope, *et al.*, *JCP*, 2006 studied under conditions considered by us, *JCP*, 2009.
- We, with A. N. al-Khateeb, have stretching-based diagnostics.
- Preliminary results indicate we have here a SACIM.

A question which extends beyond combustion!

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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.

3. Conclusions

The question as to just how the slow manifold ought to be defined seems to be presently unsettled. The procedure in J defines a unique manifold S that is slow but not strictly invariant, since orbits leave S when they leave the region of convergence. When S is extended to become S^*, it becomes invariant, but then it is no longer slow. Stated otherwise, a manifold that is locally invariant and locally slow exists but one that is globally invariant and globally slow does not. Whether such a statement would be true for other primitive equation systems presumably cannot be discovered without further work. We note, incidentally, that neither S nor S^* appears to be fuzzily defined.

More generally, Eqs. (1) are typical of innumerable systems encountered in fluid dynamics and other fields,

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!