On the potential failure of reduced reaction kinetics

J. M. Powers and S. Paolucci

Department of Aerospace and Mechanical Engineering
Department of Applied and Computational Mathematics and Statistics
University of Notre Dame, USA

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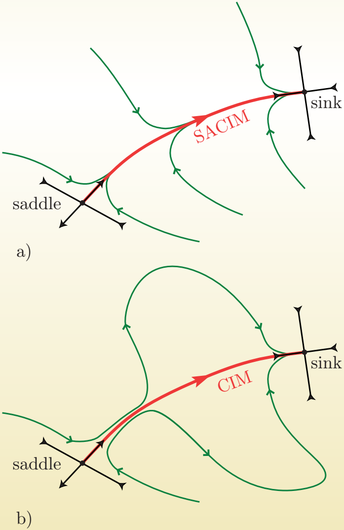
Some motivating questions...

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

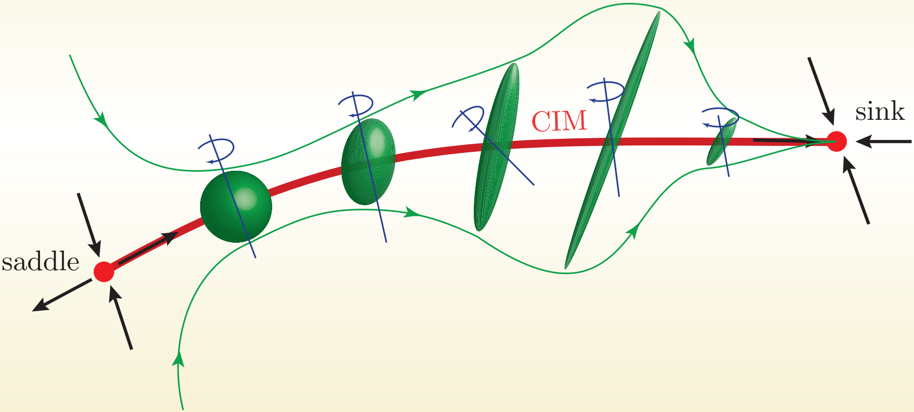
- Just what is a *SACIM*?:
  - Slow,
  - Attracting,
  - Canonical,
  - Invariant,
  - Manifold.
- Does it exist?
- Is it easy to identify?
- Does it actually work?

SACIM construction strategy: heteroclinic orbit connection

- Davis and Skodje, 1999, numerically integrate 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.



Sketch of a volume locally traversing a nearby CIM



Analogous to fluid kinematics, 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

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

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.

Procedure for local SACIM identification

- For $d\mathbf{z}/dt = \mathbf{f}(\mathbf{z})$, identify all equilibria $\mathbf{f}(\mathbf{z}) = \mathbf{0}$.
- Determine and evaluate $\mathbf{J}$ near each equilibrium to determine its source, sink, saddle, etc. character.
- Numerically integrate from candidate saddles into the unique sink to determine a CIM, $\mathbf{z}_{CIM}$, which is a candidate SACIM.
- Determine the unit tangent: $\boldsymbol{\alpha}_t = \mathbf{f}(\mathbf{z}_{CIM})/||\mathbf{f}(\mathbf{z}_{CIM})||$.
- Determine the tangential stretching rate $\sigma_t = \boldsymbol{\alpha}_t^T \cdot \mathbf{J}_s \cdot \boldsymbol{\alpha}_t$.
- Use a Gram-Schmidt procedure to identify $N-1$ unit normal vectors, thus forming an orthonormal basis.
- 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 $(N-1)\times(N-1)$ Jacobians $\mathbf{J}_{ns}$ and $\mathbf{J}_{na}$ for the motion in the hyperplane normal to the CIM:

$$\mathbf{J}_{ns} = \mathbf{Q}_n^T \cdot \mathbf{J}_s \cdot \mathbf{Q}_n, \quad \mathbf{J}_{na} = \mathbf{Q}_n^T \cdot \mathbf{J}_a \cdot \mathbf{Q}_n.$$

- Find the eigenvalues and eigenvectors of $\mathbf{J}_{ns}$. The eigenvalues give the extreme values of normal stretching rates $\sigma_{n,i}$, $i = 1, \ldots, N-1$. The normalized eigenvectors of $\mathbf{J}_{ns}$ 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 $||\mathbf{J}_{na}||$, (and $\boldsymbol{\omega}$ if 3d).

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

- By inspection, $\boldsymbol{\alpha}_t = (1,0,0)^T$.
- 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.: $\mathbf{J}_{ns}$ and $\sigma_{n,i}$

- The reduced symmetric Jacobian for the normal hyperplane is

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

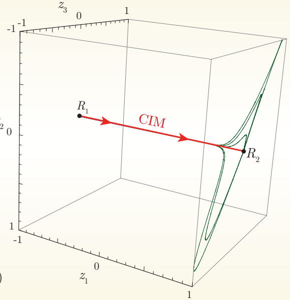
- The eigenvalues of $\mathbf{J}_{ns}$ give $\sigma_{n,i}$:

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

- $\sigma_{n,1} \sim 1$ for $z_1 \in [-1, 1]$; potential divergence from CIM.
- $\sigma_{n,2} \sim -2$ for $z_1 \in [-1, 1]$.
- $\max_i |\sigma_{n,i}|/\sigma_t \sim 10$; thus, the CIM is slow.
- $|\boldsymbol{\omega}| \sim \sigma_{n,1} \sim 1$: 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 may not be a SACIM!

- There are regions of the CIM which do not attract nearby trajectories.
- 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, $|\boldsymbol{\omega}| \sim 1$.
- But enhancement of local rotation converts the CIM into a SACIM.



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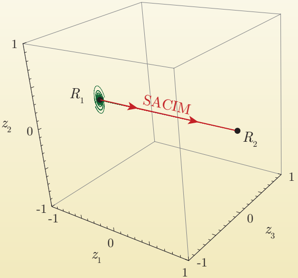
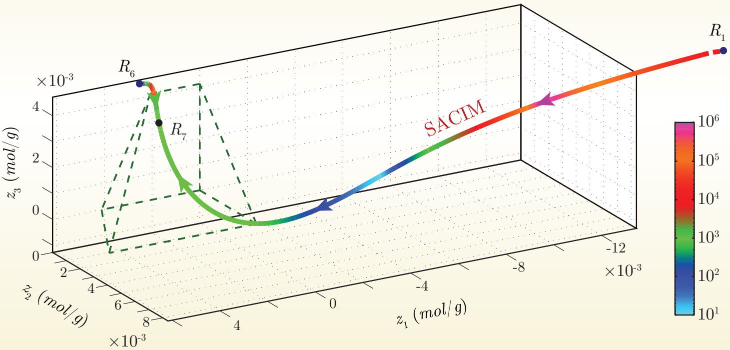


Extension to H_2-air kinetics



- Six species model of Ren, Pope, *et al.*, *JCP*, 2006 studied under conditions considered by us, *JCP*, 2009.
- For this case, we have here a SACIM.

Conclusions and questions

- The fundamental question of slow manifold identification 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?