Dynamical structure and its uses for insight, discovery, and control

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MultiSTEPS: MultiScale Transport in Environmental & Physiological Systems, IGERT www.multisteps.ictas.vt.edu
Motivation: application to data

- **Dynamical structure**: how phase space is connected / organized
- Fixed points, periodic orbits, or other invariant sets and their stable and unstable manifolds organize phase space
- Many systems defined from data or large-scale simulations — experimental measurements, observations
- e.g., from fluid dynamics, biology, social sciences
- Other tools (probabilistic, networks) could be useful in some settings
Phase space transport in 4+ dimensions

- Two examples
  - a biomechanical system
  - escape from a multi-dimensional potential well

- Then some examples from fluids and agriculture
Flying snakes

Joint work with Farid Jafari, Jake Socha, Pavlos Vlachos
Flying snakes

**Ballistic dive:**
- Jumping take-off.
- Peak glide angle of about 60°

- Lowers head.
- Organizes body into S-shape.
- Gains speed

**Shallowing glide:**
- Large-amplitude undulations.
- Glide angle of 15°-35°

Krishnan, Socha, Vlachos, Barba [2014] Physics of Fluids
Flying snakes: undulation

Krishnan, Socha, Vlachos, Barba [2014] Physics of Fluids
Flying snakes: experimental trajectories

Socha [2011] Integrative and Comparative Biology
Flying snakes: velocity space

Socha [2011] Integrative and Comparative Biology
Flying snakes: minimal model

Consider a minimal model capturing the essential coupled translational-rotational dynamics — an undulating tandem wing configuration.

Given by 4-dimensional time-periodic system

\[
\begin{align*}
\dot{v}_x &= u_1(\theta, \Omega, v_x, v_z, t) \\
\dot{v}_z &= u_2(\theta, \Omega, v_x, v_z, t) \\
\dot{\theta} &= u_3(\Omega) = \Omega \\
\dot{\Omega} &= u_4(\theta, \Omega, v_x, v_z, t)
\end{align*}
\]

with translational kinematics \( \dot{x} = v_x, \dot{z} = v_z \).

System is passively stable in pitch \( \theta \) with equilibrium manifold \( \{ \Omega = 0 \} \).

Translational dynamics are more complicated, but there does seem to be a ‘shallowing manifold’.

Flying snakes: achieving equilibrium glide
Flying snakes: falling like a stone
Flying snakes: separatrix behavior

saddle-node bifurcation at $\theta^*$ along shallowing manifold
Ship motion and capsize
Tubes leading to capsize

- Model built around Hamiltonian,
  \[ H = \frac{p_x^2}{2} + R^2 p_y^2/4 + V(x, y), \]
  where \( x = \text{roll} \) and \( y = \text{pitch} \) are coupled

\[ V(x, y) \]

\[ E < E_c \]

\[ E > E_c \]
Tubes leading to capsize

Poincare section

transition state
Tubes leading to capsize

• Wedge of trajectories leading to imminent capsize

• Tubes are a useful paradigm for predicting capsize even in the presence of random forcing, e.g., random ocean waves

• Could inform control schemes to avoid capsize in rough seas
2D fluid example – almost-cyclic behavior

- A microchannel mixer: microfluidic channel with spatially periodic flow structure, e.g., due to grooves or wall motion\(^1\)
- How does behavior change with parameters?

\(^1\)Stroock et al. [2002], Stremler et al. [2011]
2D fluid example – almost-cyclic behavior

- A microchannel mixer: modeled as periodic Stokes flow

![Streamline patterns](image)

- piecewise constant vector field (repeating periodically)
  - top streamline pattern during first half-cycle (duration $\tau_f/2$)
  - bottom streamline pattern during second half-cycle (duration $\tau_f/2$), then repeat

- System has parameter $\tau_f$, period of one cycle of flow, which we treat as a bifurcation parameter — there’s a critical point $\tau_f^* = 1$
2D fluid example – almost-cyclic behavior

- Poincaré section for $\tau_f < 1 \Rightarrow$ no obvious structure!

- Poincaré map: Over large range of parameter, no obvious cyclic behavior
- So, is the phase space featureless?
Almost-invariant sets / almost-cyclic sets

- No, we can identify **almost-invariant sets** (AISs) and **almost-cyclic sets** (ACSs)\(^1\)
- Create box partition of phase space \(\mathcal{B} = \{B_1, \ldots B_q\}\), with \(q\) large
- Consider a \(q\)-by-\(q\) **transition (Ulam) matrix**, \(P\), where

\[
P_{i,j} = \frac{m(B_i \cap f^{-1}(B_j))}{m(B_i]},
\]

the transition probability from \(B_i\) to \(B_j\) using, e.g., \(f = \phi_{t+T}^t\), often computed numerically

- \(P\) approximates \(\mathcal{P}\), Perron-Frobenius transfer operator — which evolves densities, \(\nu\), over one iterate of \(f\), as \(\mathcal{P}\nu\)
- Typically, we use a reversibilized operator \(R\), obtained from \(P\)

\(^1\)Dellnitz & Junge [1999], Froyland & Dellnitz [2003]
Identifying AISs by graph- or spectrum-partitioning

- $P$ admits graph representation where nodes correspond to boxes $B_i$ and transitions between them are edges of a directed graph.
- Graph partitioning methods can be applied\(^1\)
- can obtain AISs/ACSs and transport between them
- spectrum-partitioning as well (eigenvectors of large eigenvalues)\(^2\)

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\(^1\)Dellnitz, Junge, Koon, Lekien, Lo, Marsden, Padberg, Preis, Ross, Thiere [2005] Int. J. Bif. Chaos
\(^2\)Dellnitz, Froyland, Sertl [2000] Nonlinearity
Identifying AISs by graph- or spectrum-partitioning

Top eigenvectors of transfer operator reveal structure

$v_2$

$v_3$

$v_4$

$v_5$

$v_6$
Almost-cyclic sets stir fluid like rods

The zero contour (black) is the boundary between the two almost-invariant sets.

- Three-component AIS made of 3 ACSs each of period 3
Almost-cyclic sets stir fluid like rods

Almost-cyclic sets, in effect, stir the surrounding fluid like ‘ghost rods’

In fact, there’s a theorem (Thurston-Nielsen classification theorem) that provides a topological lower bound on the mixing based on braiding in space-time
Almost-cyclic sets stir fluid like rods

Thurston-Nielsen theorem applies only to periodic points
— But seems to work, even for approximately cyclic blobs of fluid\textsuperscript{1}

Eigenvalues/eigenvectors vs. parameter

Top eigenvalues of transfer operator as parameter $\tau_f$ changes

Lines colored according to continuity of eigenvector
Genuine eigenvalue crossings? Eigenvalues generically avoid crossings if there is no symmetry present (Dellnitz, Melbourne, 1994)
Eigenvalues/eigenvectors vs. parameter

change in eigenvector along thick red branch (a to f), as $\tau_f$ decreases.

Grover, Ross, Stremler, Kumar [2012] Chaos
Predict critical transitions in geophysical transport?

Ozone data (Lekien and Ross [2010] Chaos)
Predict critical transitions in geophysical transport?

- Different eigenmodes can correspond to dramatically different behavior.
- Some eigenmodes increase in importance while others decrease.
- Can we predict dramatic changes in system behavior?
- e.g., predicting major changes in geophysical transport patterns?
Chaotic fluid transport: aperiodic setting

- Identify regions of high sensitivity of initial conditions
- The finite-time Lyapunov exponent (FTLE),
  \[
  \sigma_t^T(x) = \frac{1}{|T|} \log \| D\phi_t^{t+T}(x) \|
  \]
  measures the maximum stretching rate over the interval $T$ of trajectories starting near the point $x$ at time $t$
- Ridges of $\sigma_t^T$ reveal hyperbolic codim-1 surfaces; finite-time stable/unstable manifolds; ‘Lagrangian coherent structures’ or LCSs$^2$

$^2$ cf. Bowman, 1999; Haller & Yuan, 2000; Haller, 2001; Shadden, Lekien, Marsden, 2005
Repelling and attracting structures

- attracting structures for $T < 0$
- repelling structures for $T > 0$

Peacock and Haller [2013]
Repelling and attracting structures

- Stable manifolds are repelling structures
- Unstable manifolds are attracting structures

Peacock and Haller [2013]
Atmospheric flows: continental U.S.

LCSs: orange = repelling, blue = attracting
2D curtain-like structures bounding air masses
Atmospheric flows and lobe dynamics

orange = repelling LCSs, blue = attracting LCSs

Andrea, first storm of 2007 hurricane season

Atmospheric flows and lobe dynamics

Andrea at one snapshot; LCS shown (orange = repelling, blue = attracting)
Atmospheric flows and lobe dynamics

orange = repelling (stable manifold),    blue = attracting (unstable manifold)
Atmospheric flows and lobe dynamics

orange = repelling (stable manifold), blue = attracting (unstable manifold)
Atmospheric flows and lobe dynamics

Portions of lobes colored; magenta = outgoing, green = incoming, purple = stays out
Atmospheric flows and lobe dynamics

Portions of lobes colored; magenta = outgoing, green = incoming, purple = stays out
Atmospheric flows and lobe dynamics

Sets behave as lobe dynamics dictates
Airborne diseases moved about by coherent structures

Joint work with David Schmale, Plant Pathology / Agriculture at Virginia Tech
Coherent filament with high pathogen values

12:00 UTC 1 May 2007

15:00 UTC 1 May 2007

18:00 UTC 1 May 2007

Coherent filament with high pathogen values

12:00 UTC 1 May 2007  15:00 UTC 1 May 2007  18:00 UTC 1 May 2007

Laboratory fluid experiments

3D Lagrangian structure for non-tracer particles:
— Inertial particle patterns (do not follow fluid velocity)

e.g., allows further exploration of physics of multi-phase flows

\[^3\text{Raben, Ross, Vlachos [2014,2015] Experiments in Fluids}\]
Detecting causality

- Ultimate goal: detecting causality between two time series,

\[\text{I would rather discover one causal law than be King of Persia.}\]
Democritus (460-370 B.C.)
Detecting causality

• We have just two time series,
  – Which signal is the driver,
  – Causality direction, \( X \rightarrow Y \) \( X \leftarrow Y \)
  – Direct causality vs. common external forcing,
  – ...

• Signals from:
  – Measurements: temperature, pressure, salinity, velocity, ...
  – Maps,
  – ODE’s, PDE’s, ...
Detecting causality – cross-mapping approach

• If two signals are from a same n-D manifold, then there would be some correspondence between shadow manifolds (reconstructed phase spaces),

Estimating states across manifolds using nearest neighbors:

• If x(t) causally influences y(t) then signature of x(t) inherently exists in y(t),

\[
\dot{y}(t) = \bar{f}(x, y, ...) \\
y(t + 1) = \bar{g}(x(t), y(t))
\]

• If so, historical record of y(t) values can reliably estimate the state of x

Sugihara et al. 2012
Detecting causality – agricultural example

Determining the causal network via nonlinear state space reconstruction and convergent cross mapping
Phase space geometry — looking forward

Many inter-related concepts

- apply to data-based finite-time settings — just more interesting
- almost-invariant sets, almost-cyclic sets, braids, LCS, transfer operators, phase space transport networks, dependence on parameters, separatrices, basins of stability

Opportunities:

- use in control
- value-added way of viewing and comparing data
- detecting causality

Applications:

- agriculture, ecology
- predicting critical transitions in geophysical flow patterns
- comparative biomechanics, ...