Exact coherent structures in turbulence: framework, numerics, and questions

John F. Gibson

Integrated Applied Mathematics
Mathematics & Statistics
University of New Hampshire

UNH Workshop on High-Re Boundary Layer Turbulence
20 November 2015

alternate title

Yes, you can do bifurcation analysis of a DNS

Outline

I Conceptual framework: *low-d dynamical systems*

II Numerical methods: *Newton-Krylov-hookstep*

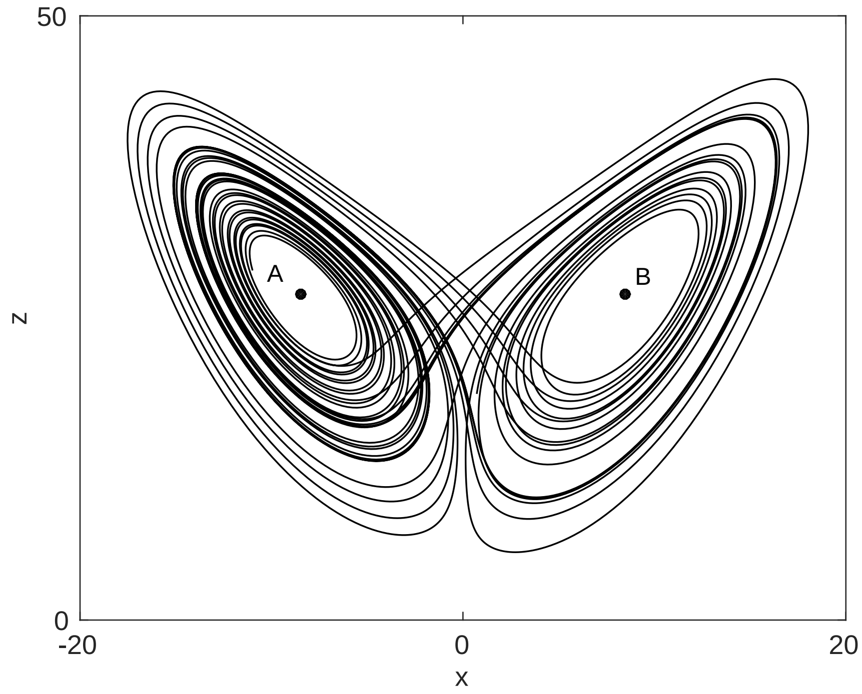
III Survey of results: *mostly mine*

IV Questions and future directions

Conceptual framework

low-d dynamical systems

Lorenz system

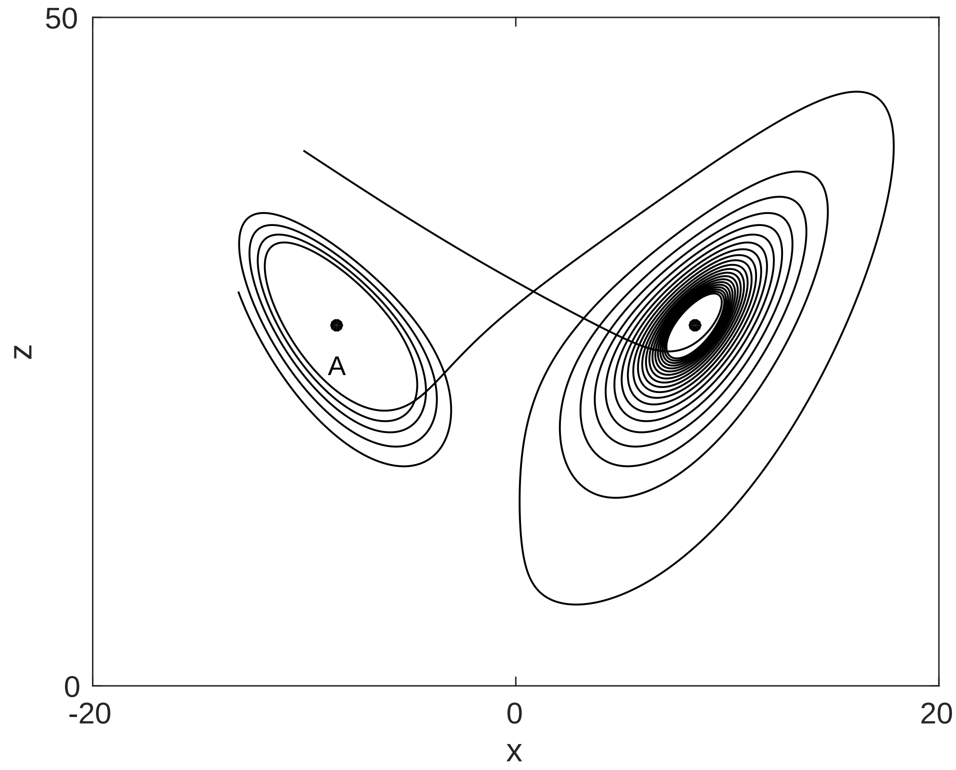


$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = \rho x - y - xz$$
$$\dot{z} = -\beta z + xy, \qquad \sigma = 10,\ \beta = 8/3,\ \rho = 28$$

Equilibria at origin and

$$A, B = (\pm\sqrt{\beta(\rho-1)},\ \pm\sqrt{\beta(\rho-1)},\ \rho - 1) \doteq (\pm 8.48,\ \pm 8.48,\ 27)$$

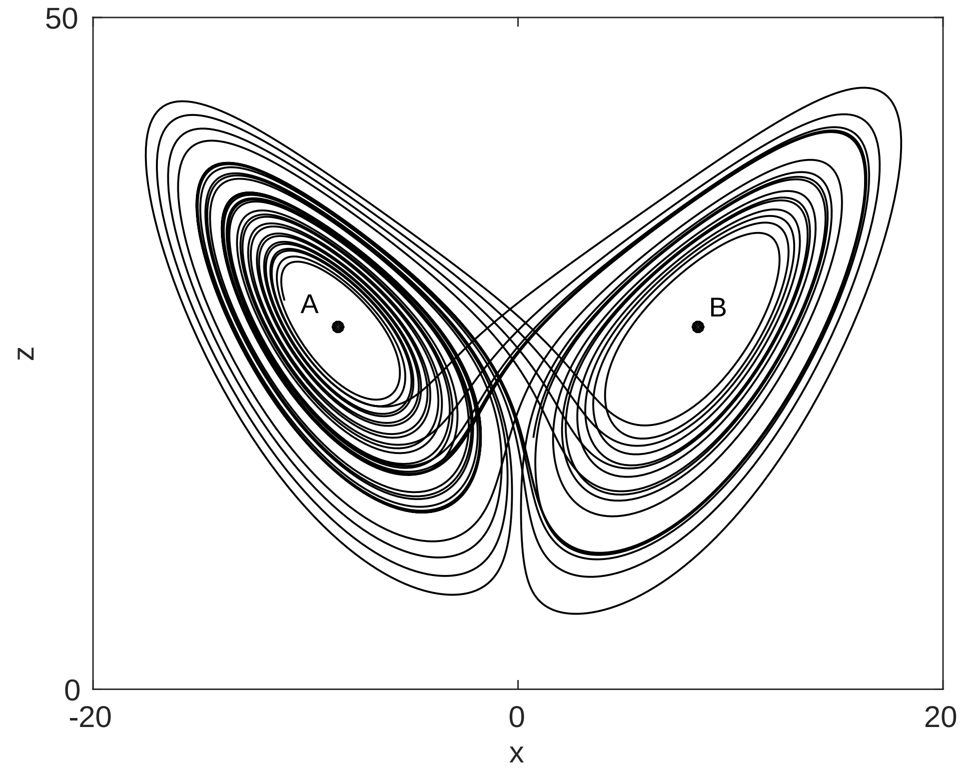
Lorenz system



Eigenvalues at A,B

$$\lambda_1 = -13.8$$
$$\lambda_{2,3} = 0.094 \pm 10.2\, i$$

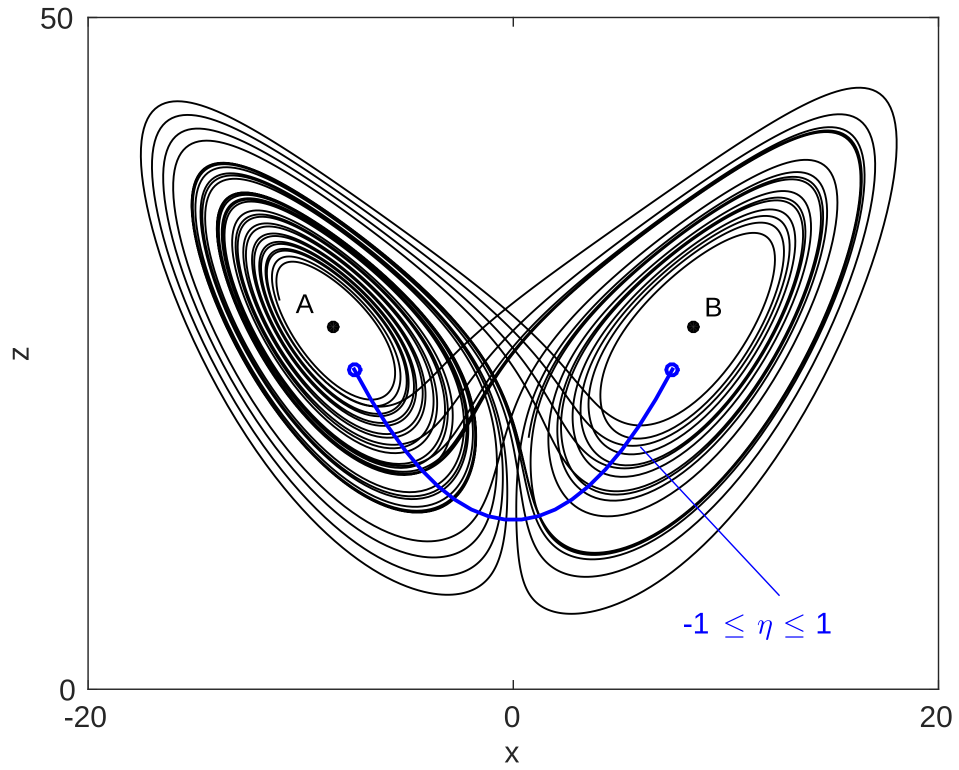
Lorenz system



Equilibria organize the dynamics but are not part of the attractor.

The attractor is best characterized by its periodic orbits.

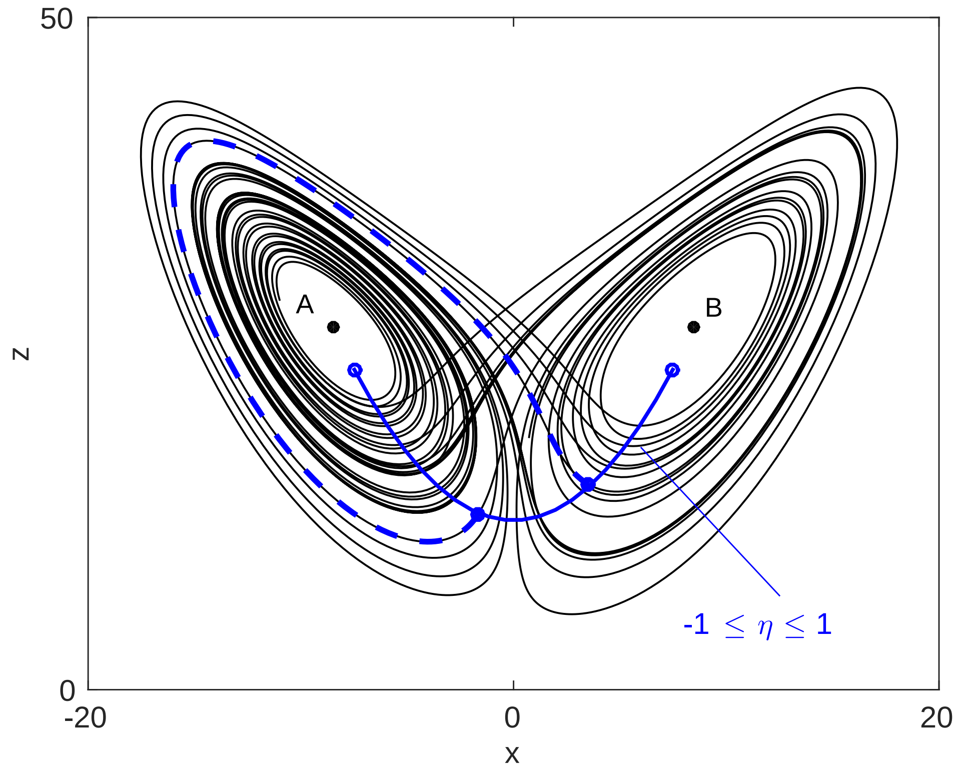
How to find the periodic orbits of Lorenz



Construct 1-d Poincare section on nearly 2-d surface of attractor.

Parameterize as $-1 \leq \eta \leq 1$.

Lorenz: Poincare map

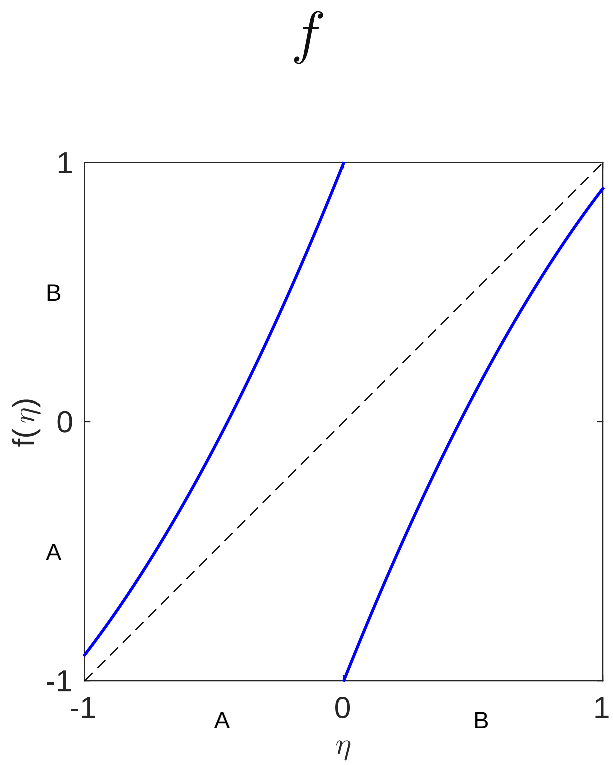


Flow induces map from $-1 \leq \eta \leq 1$ onto itself: $\eta_{n+1} = f(\eta_n)$.

Associate $-1 \leq \eta < 0$ with A and $0 < \eta \leq 1$ with B.

Note discontinuity of map at $\eta = 0$.

Lorenz Poincare map, 1st iterate



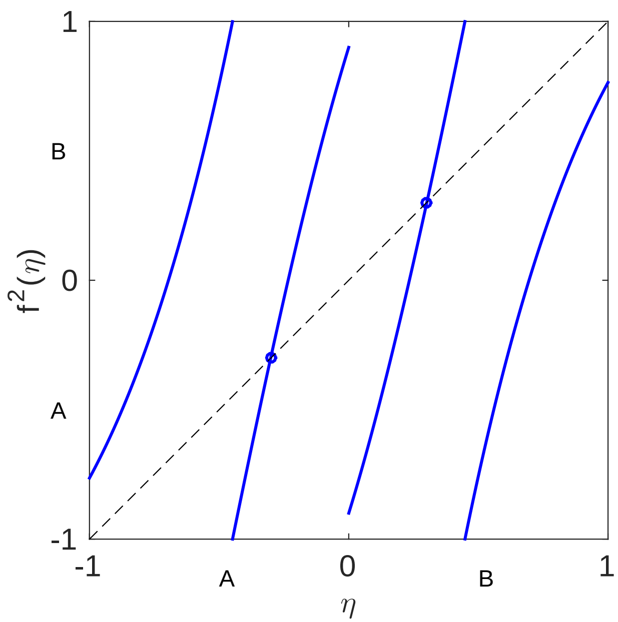
Graph of f mapping η onto itself: $\eta_{n+1} = f(\eta_n)$.

Period-1 orbit would have $\eta_{n+1} = f(\eta_n) = \eta_n$.

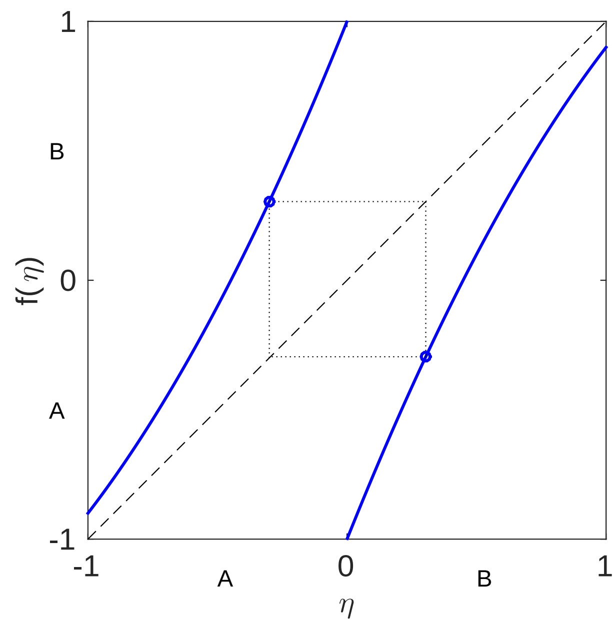
No intersections of $f(\eta)$ with identity $\Rightarrow$ no period-1 orbits.

Lorenz Poincare map, 2nd iterate

$$f^2(\eta) = f(f(\eta))$$



$$f$$

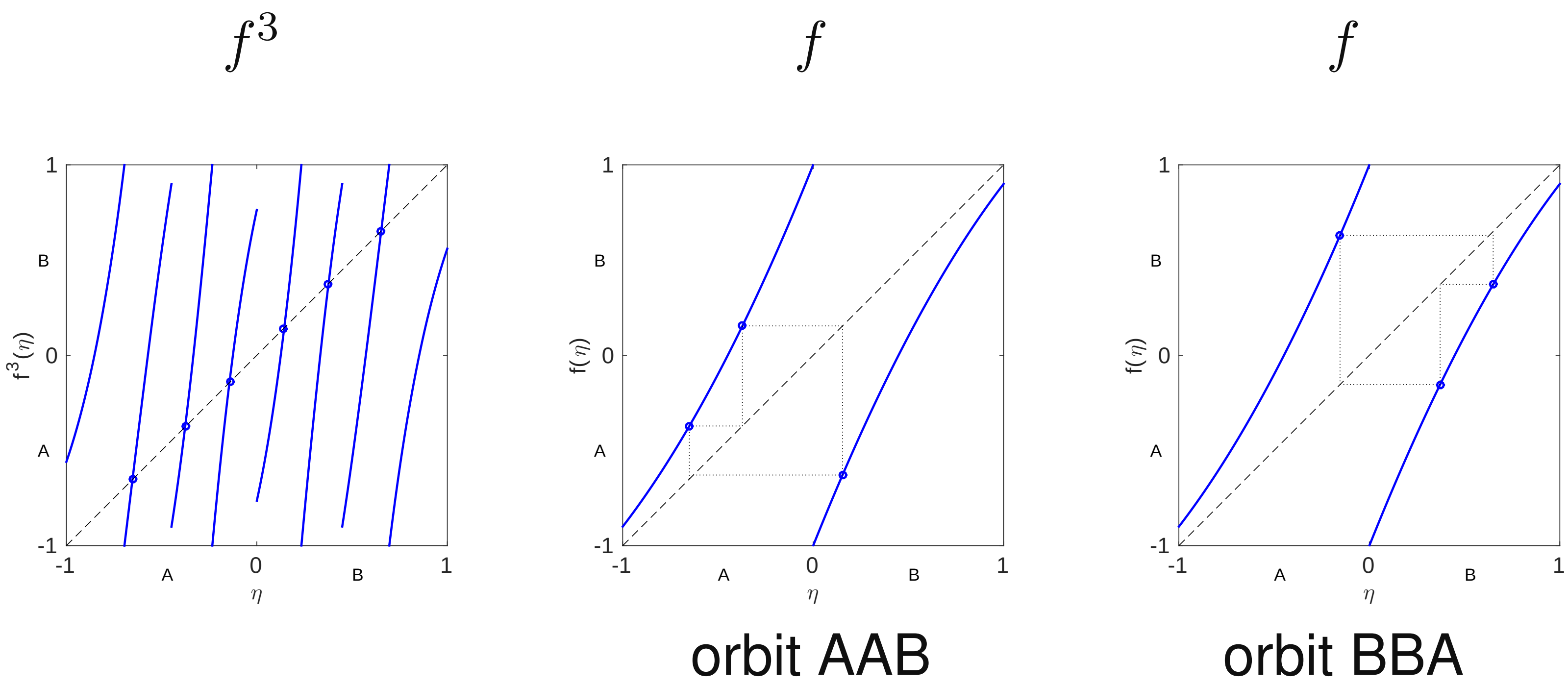


periodic orbit AB

2nd iterate $\eta_{n+2} = f^2(\eta_n)$ intersects identity at two points.

$\Rightarrow$ one period-2 orbit $\eta = f^2(\eta)$, symbol sequence AB AB AB AB $\ldots$

Lorenz Poincare map, 3rd iterate



3rd iterate $\eta_{n+3} = f^3(\eta_n)$ intersects identity at six points.

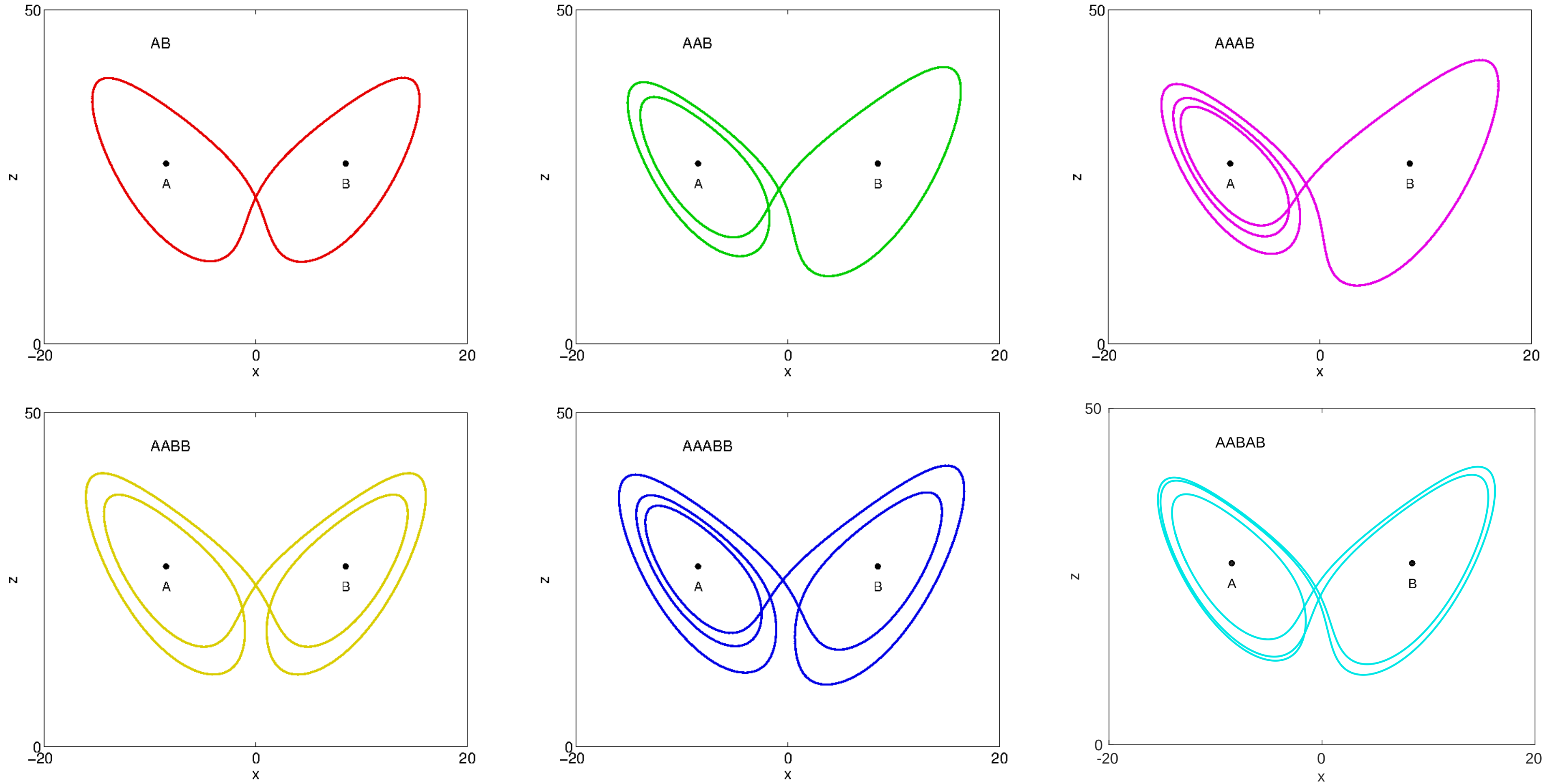
$\Rightarrow$ two period-3 orbits $\eta = f^3(\eta)$, symbol sequences

AAB AAB AAB AAB $\ldots$ and BBA BBA BBA BBA $\ldots$

Find all 11101 period-n orbits and n-length symbol for $n \leq 20$ *

* Viswanath (2008) Nonlinearity

Lorenz: periodic orbits

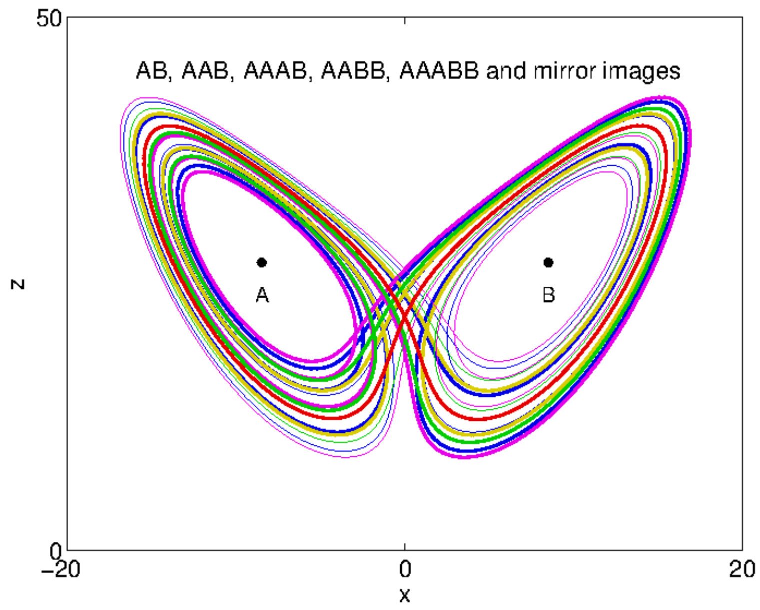


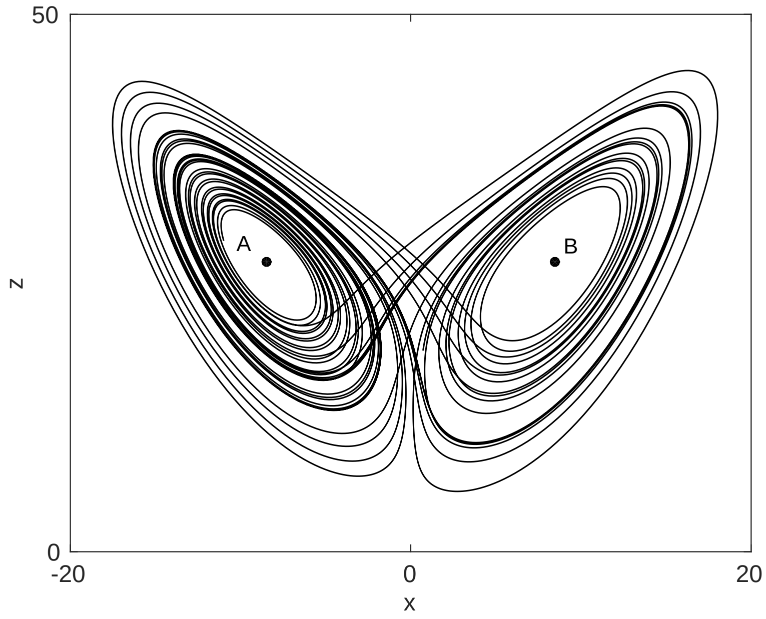
Countably infinite set of periodic orbits, ordered by length and instability

---

Viswanath (2008) Nonlinearity

Lorenz: ensemble of periodic orbits





Periodic orbits

- unstable, countably infinite, ordered by length or instability
- dense in attracting set ($\exists$ orbit arbitrarily close to any point on attractor)
- chaotic attractor is limit set of its unstable periodic orbits

Periodic Orbit Theory

Theoretical framework for analyzing chaotic attractors

properties of unstable orbits $\Rightarrow$ time-avg statistics

Nonlinear ODEs induce linear PDEs on probability density functions

$$f^t : x(0) \to x(t) \quad \Rightarrow \quad e^{t\mathcal{A}} : \rho(x,0) \to \rho(x,t)$$

Invariant measure $=$ eigenfunction ρ of $e^{t\mathcal{A}} = \sum$ nbrhds of periodic orbits of f

Expansions produce *trace formulae* relating time averages to sums over orbits

$$\int_0^\infty e^{-st}\,\mathrm{tr}\, e^{t\mathcal{A}}\, dt = \mathrm{tr}\,\frac{1}{s-\mathcal{A}} = \sum_{\text{orbits } p} T_p \sum_{r=1}^\infty \frac{e^{-sT_p r}}{|\det(I - Df_{\perp,p}^{T_p r})|}$$

Convergence is superexponential, but requires *all* orbits up to given period T

Ruelle, Gutzwiller, Cvitanović, . . .

`www.chaosbook.org`

Numerical methods

can we do this for fluids?

Issues with fluids

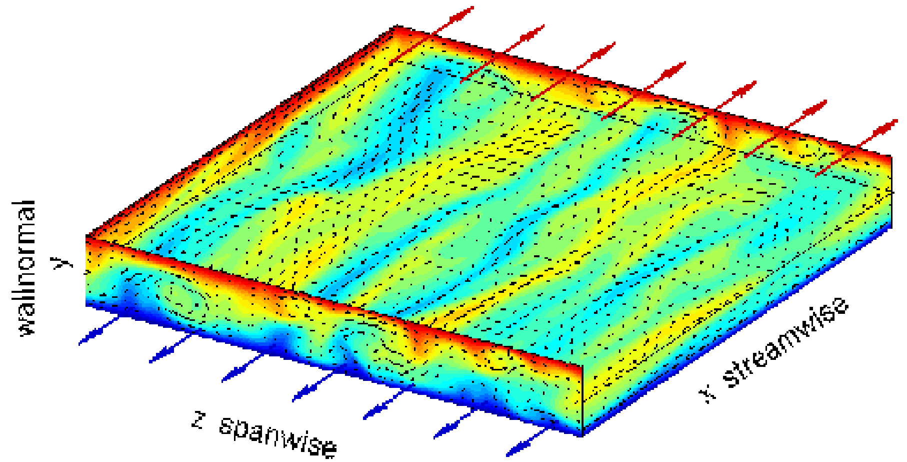
Problems

- Infinite dimensionality, in practice very high-d numerics
- No symbolic dynamics to guide initial guesses for orbits
- Is Navier-Stokes regular? Hyperbolic?

On the other hand,

- Viscosity strongly contracts high-order modes
- Coherent structures suggest low-d organization
- Fast & accurate numerical simulation methods
- Blaze ahead without theoretical justification

Plane Couette flow



Navier-Stokes, BCs

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \boldsymbol{\nabla} \mathbf{u} = -\boldsymbol{\nabla} p + \frac{1}{Re} \nabla^2 \mathbf{u}$$

$$\boldsymbol{\nabla} \cdot \mathbf{u} = 0$$

$$\mathbf{u}(x + L_x, y, z) = \mathbf{u}(x, y, z + L_z) = \mathbf{u}(x, y, z), \quad \mathbf{u}(x, \pm 1, z) = \pm 1$$

Represent time evolution under Navier-Stokes as

$$\boxed{\mathbf{u}(t) = f^t(\mathbf{u}(0))}$$

Problem formulation

Seek four types of **invariant solutions**

$$
\begin{aligned}
f^t(\mathbf{u}) &= \mathbf{u}, && \forall t && \text{equilibrium} \\
f^t(\mathbf{u}) &= \tau(t)\mathbf{u}, && \forall t && \text{traveling wave} \\
f^t(\mathbf{u}) &= \mathbf{u}, && t = T, 2T, 3T, \ldots && \text{periodic orbit} \\
f^t(\mathbf{u}) &= \sigma\mathbf{u}, && t = T, 2T, 3T, \ldots && \text{relative periodic orbit}
\end{aligned}
$$

where

$$
\begin{aligned}
f^t &= \text{time integration of Navier-Stokes} \\
\sigma &= \text{symmetry of Navier-Stokes and BCs} \\
\tau(t) &= \text{phase shift, e.g. } \tau(t)\mathbf{u}(x, y, z) = \mathbf{u}(x - c_x t, y, z - c_z t)
\end{aligned}
$$

General invariance equation:

$$\boxed{g(\mathbf{u}, T, \sigma) = f^T(\mathbf{u}) - \sigma\mathbf{u} = 0}$$

Numerical formulation

- Periodic orbit satisfies

$$g(\mathbf{u}, T) = f^T(\mathbf{u}) - \mathbf{u} = 0 \qquad (f^t = \text{evolution by Navier-Stokes})$$

- Discretize $\mathbf{u}$ with spectral expansion

$$\mathbf{u}(\mathbf{x}, t) = \sum_{j,k,\ell} \hat{\mathbf{u}}_{jk\ell}(t)\; T_\ell(y)\; e^{2\pi i (jx/L_x + kz/L_z)}$$

- Discretize f^t with semi-implicit finite-diff time stepping (DNS)
- Nonlinear eqn in $O(10^5)$ to $O(10^6)$ unknowns $\hat{\mathbf{u}}_{jk\ell}, T$
- Solve with Newton-Kylov-hookstep algorithm of Viswanath, 2007.

Computing periodic orbits: Newton method

Find periodic orbit $\mathbf{u}^*, T^*$ solution of $g(\mathbf{u}^*, T^*) = 0$

- Start with guess $(\mathbf{u}, T)$ near solution $(\mathbf{u}^*, T^*)$

$$\mathbf{u}^* = \mathbf{u} + \delta\mathbf{u}, \quad T^* = T + \delta T$$

- Expand g in Taylor series

$$\begin{aligned} g(\mathbf{u}^*, T^*) &= g(\mathbf{u} + \delta\mathbf{u},\ T + \delta T) \\ 0 &= g(\mathbf{u}, T) + Dg\ (\delta\mathbf{u}, \delta T) \end{aligned}$$

- Newton-step eqn

$$\boxed{Dg\ (\delta\mathbf{u}, \delta T) = -g(\mathbf{u}, T)}$$

- Has form of $Ax = b$ problem, solve for Newton step $(\delta\mathbf{u}, \delta T)$
- Let $(\mathbf{u}, T) \to (\mathbf{u} + \delta\mathbf{u},\ T + \delta T)$ and iterate.

Solution of Newton-step eqn

Newton step eqn

$$Dg\ (\delta\mathbf{u}, \delta T) = -g(\mathbf{u}, T)$$

Problem

Dg is huge: $10^5 \times 10^5$ to $10^6 \times 10^6$

Dg is not sparse

Dg too big to evaluate: 100 GB to 10 TB

Too big to solve directly: days to years for $O(m^3)$ direct algorithm

Solution

Solve with iterative Krylov-subspace method, GMRES.

GMRES algorithm (Generalized Minimum Residuals)

Solve $m \times m$ system of eqns $Ax = b$ with $m = O(10^6)$

Define n-dimensional Krylov subspace of $\mathbb{C}^m$ for $n \ll m$

$$\begin{aligned}
K_1 &= \text{span}\{b\} \\
K_2 &= \text{span}\{b, Ab\} \\
K_3 &= \text{span}\{b, Ab, A^2b\} \\
K_n &= \text{span}\{b, Ab, A^2b, \ldots, A^{n-1}b\}
\end{aligned}$$

Note that $AK_n \subset K_{n+1}$.

Construct orthonormal basis for K_n via Gram-Schmidt orthogonalization

$$\begin{aligned}
K_1 &= \text{span}\{q_1\} \\
K_2 &= \text{span}\{q_1, q_2\} \\
K_3 &= \text{span}\{q_1, q_2, q_3\} \\
K_n &= \text{span}\{q_1, q_2, q_3, \ldots, q_n\}
\end{aligned}$$

Then $AQ_n = Q_{n+1}H_n$ where H_n is $(n+1) \times n$, and Q_n has columns $q_1, \ldots, q_n$.

GMRES iterative solution of $Ax = b$

Given $AQ_n = Q_{n+1}H_n$ for $(n+1) \times n$ H_n and cols of Q_n span K_n

The following minimization problems are equivalent

min $\|Ax_n - b\|_2$ over $x_n \in K_n$

min $\|AQ_n y_n - b\|_2$ over $y_n \in \mathbb{C}^n$

min $\|Q_{n+1}H_n y_n - b\|_2$ over $y_n \in \mathbb{C}^n$

min $\|H_n y_n - Q_{n+1}^* b\|_2$ over $y_n \in \mathbb{C}^n$

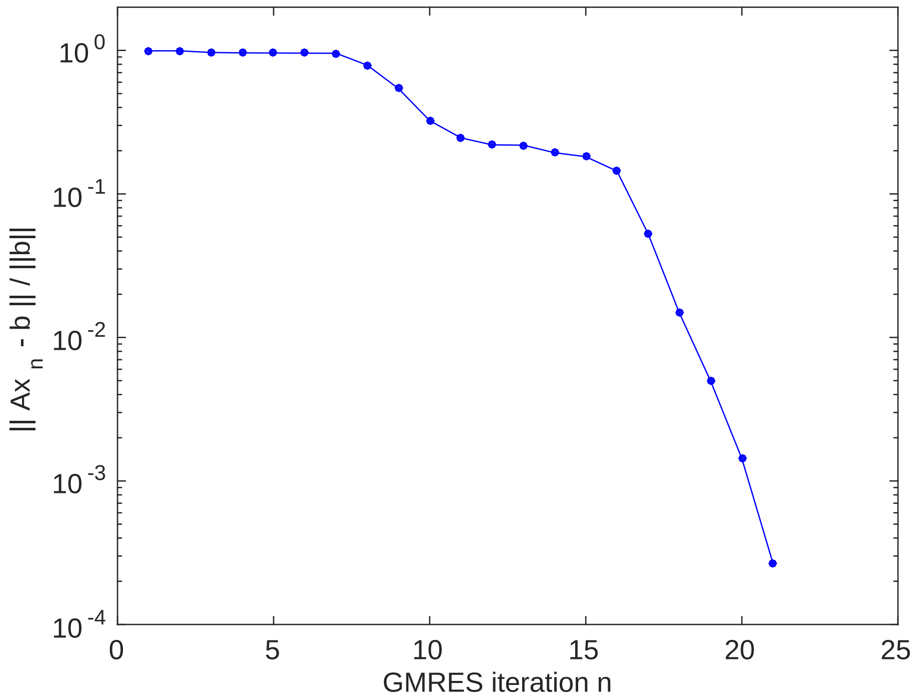
Last equation is low-d least-squares problem, $(n+1) \times n$ for $n \ll m$.

Given solution y_n, approximate solution to $Ax = b$ is $x_n = Q_n y_n$.

$K_n =$ span$\{b, Ab, A^2b, \ldots, A^{n-1}b\}$ aligns with leading eigenspace of A.

Thus x_n converges quickly if b is dominated by leading eigenspace of A.

GMRES convergence



Computation of Newton step for periodic orbit of plane Couette flow

- $m = 2 \cdot 48^3 \approx 10^5$ unknowns
- periodic orbit has 3 unstable eigenvalues
- **Newton step converges to 10^{-3} accuracy in $n = 20$ iterations**

GMRES as a "matrix-free" computation

GMRES requires computation Ax for test values of x, not A itself.

For Newton-step eqn, Ax corresponds to operator on LHS

$$Dg\;(\delta\mathbf{u}, \delta T) = -g(\mathbf{u}, T)$$

Approximate LHS operation with finite-differencing

$$Dg\;(\delta\mathbf{u}, \delta T) \;\doteq\; g(\mathbf{u}+\delta\mathbf{u},\; T+\delta T) - g(\mathbf{u}, T)$$

Substitute $g(\mathbf{u}, T) = f^T(\mathbf{u}) - \mathbf{u}$

$$Dg\;(\delta\mathbf{u}, \delta T) \;\doteq\; f^{T+\delta T}(\mathbf{u}+\delta\mathbf{u}) - f^T(\mathbf{u}) - \delta\mathbf{u}$$

Each GMRES iteration takes one DNS time-integration $f^{T+\delta T}$.

No need to compute or store Dg.

Hookstep trust-region modification of Newton method

Problem: Newton step goes haywire if guess is far from solution $(\mathbf{u}^*, T^*)$

Solution: Instead of taking Newton step from Newton eqn

$$Dg\ (\delta\mathbf{u}, \delta T) = -g(\mathbf{u}, T),$$

minimize the residual of the Newton eqn

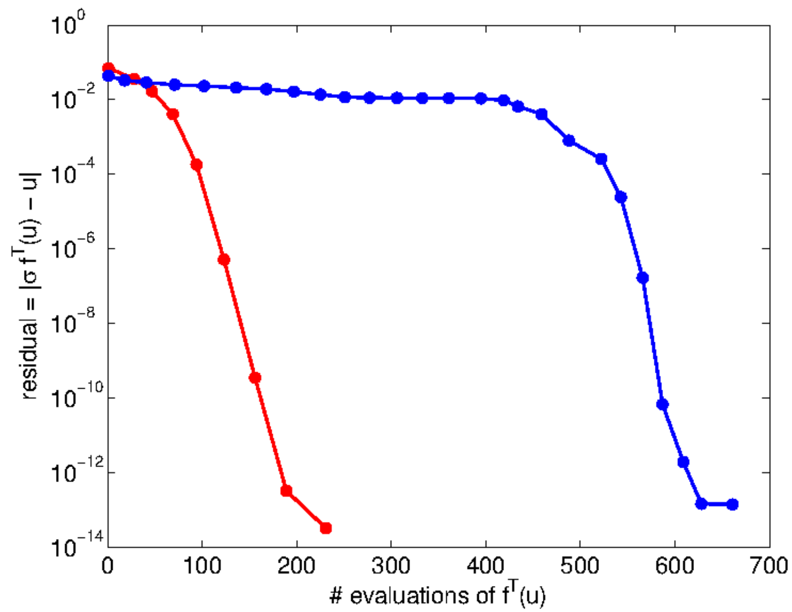
$$\|Dg\ (\delta\mathbf{u}, \delta T) + g(\mathbf{u}, T)\|_2$$

with constraints $\|(\delta\mathbf{u}, \delta T)\| \leq R$ and $(\delta\mathbf{u}, \delta T)$ in Krylov subspace

- Calculable from $(n+1) \times n$ SVD of H matrix from GMRES.
- Adjust R based on accuracy of local linearization.
- For small R, hookstep = gradient descent on Newton-eqn residual.
- For large R, hookstep = Newton step.

Viswanath (2007) JFM 580, Dennis & Schabel (1996)

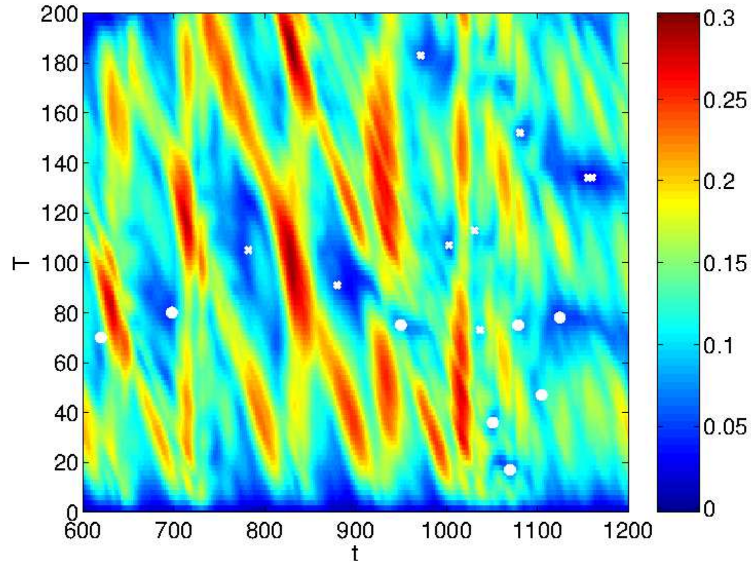
Newton-Krylov-hookstep convergence



Hookstep increases convergence region of search by orders of magnitude

- each dot is one Newton/hookstep iteration
- typical: long creep downhill (gradient) then rapid convergence (Newton)
- unusual: very good initial guess, immediate rapid convergence
- equilibria take a few CPU-hours; periodic orbits one CPU-day (minimal flows)

Initial guesses for Newton-Krylov-hookstep search



$$r(t,T) = \frac{\|\mathbf{u}(t+T)-\mathbf{u}(t)\|}{\langle \|\mathbf{u}\|^2 \rangle^{1/2}}$$

Get initial guesses $(\mathbf{u}, T)$ from close recurrences $f^T(\mathbf{u}) - \mathbf{u} \approx 0$

Compute long time series of data $\mathbf{u}(t)$ by DNS

Look for local minima of recurrence residual $\|\mathbf{u}(t+T) - \mathbf{u}(t)\|$

Circles mark guesses that converged to periodic orbits, X's mark failures.

Results

Results for plane Couette flow, minimal flow unit, $Re = 400$

- $O(20)$ equilibria, $O(50)$ periodic orbits, $O(5)$ heteroclinic connections
- Well-resolved states of DNS, dense in $\hat{\mathbf{u}}_{jk\ell}$ on 48^3 grid

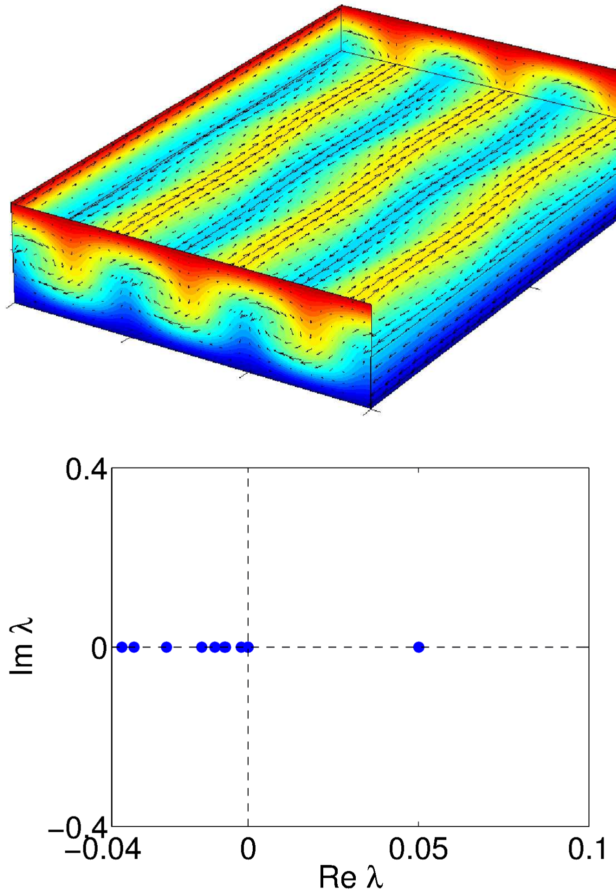
$$\mathbf{u}(\mathbf{x}) = \sum_{j,k,\ell} \hat{\mathbf{u}}_{jk\ell}\, T_\ell(y)\, e^{2\pi i(jx/L_x + kz/L_z)}$$

- Spatial resolution $O(10^{-5})$, temporal resolution $O(10^{-4})$.
- Satisfy discretized invariant equation $f^T(\mathbf{u}) - \mathbf{u} = O(10^{-13})$.
- $O(10)$ unstable eigenvalues $\lll O(10^5)$ stable eigenvalues.

Well-resolved, fully nonlinear DNS computations, no modeling.

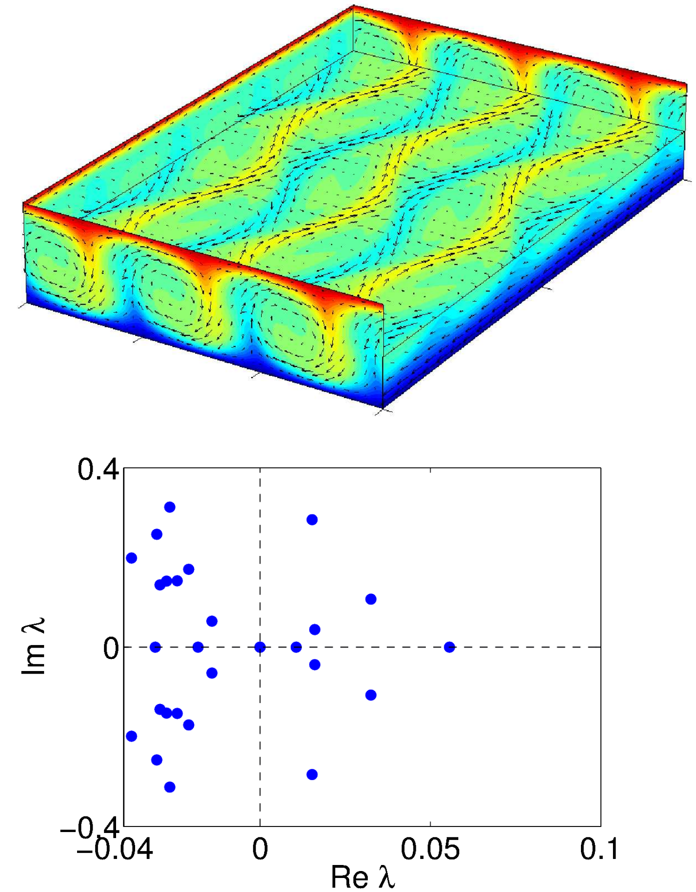
Plane Couette equilibria: Nagata, Busse, Clever, Waleffe solutions

EQ1, lower branch



1 unstable eigenvalue!

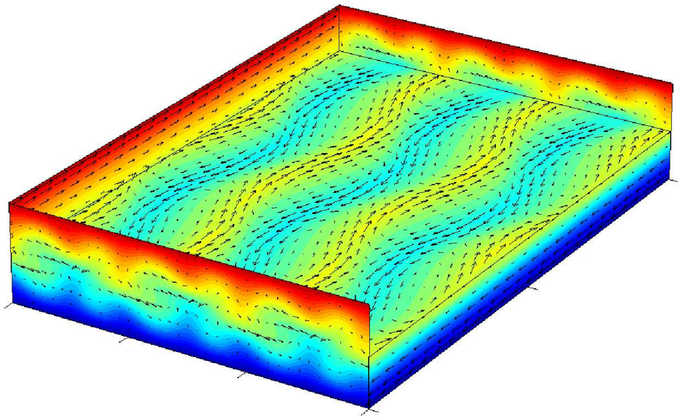
EQ2, upper branch

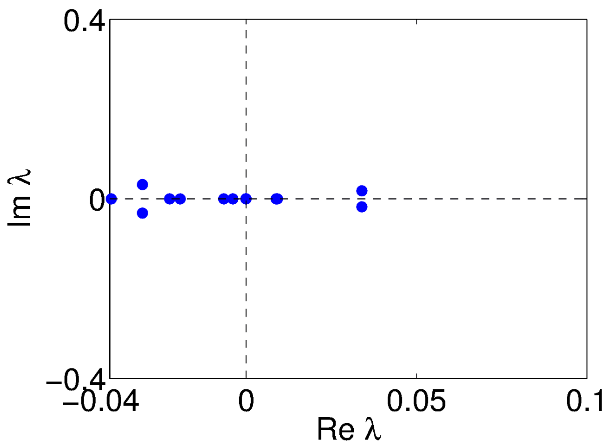


Nagata (1990) JFM 217; Clever & Busse (1997) JFM 344; Waleffe (2003) *Phys. Fluids* 15; Wang, Gibson, Waleffe (2007) PRL 98

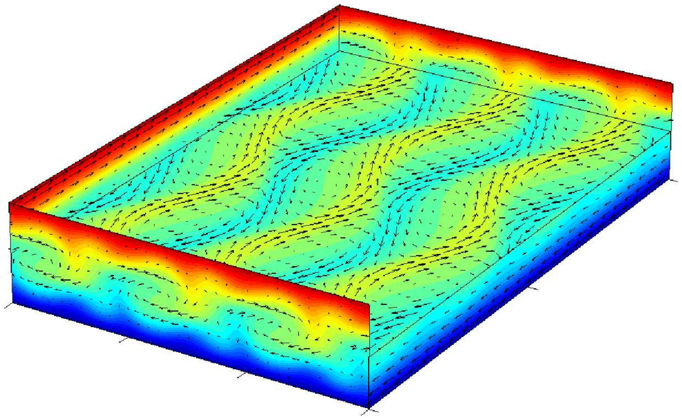
Equilibria

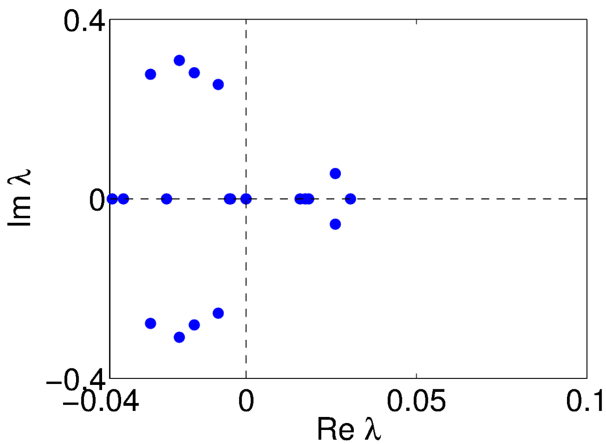
EQ3, lower branch



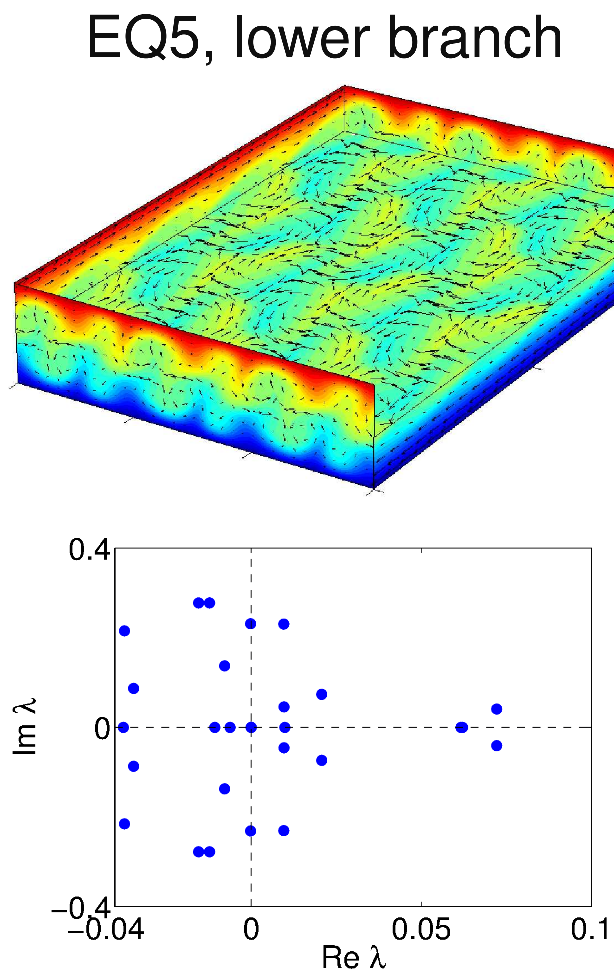


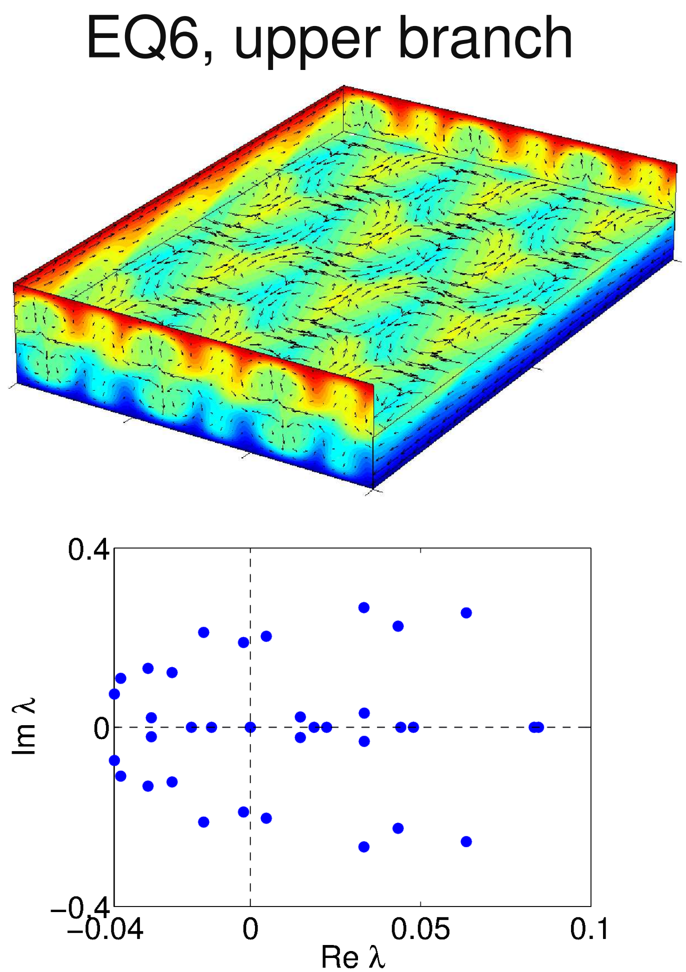
EQ4, upper branch



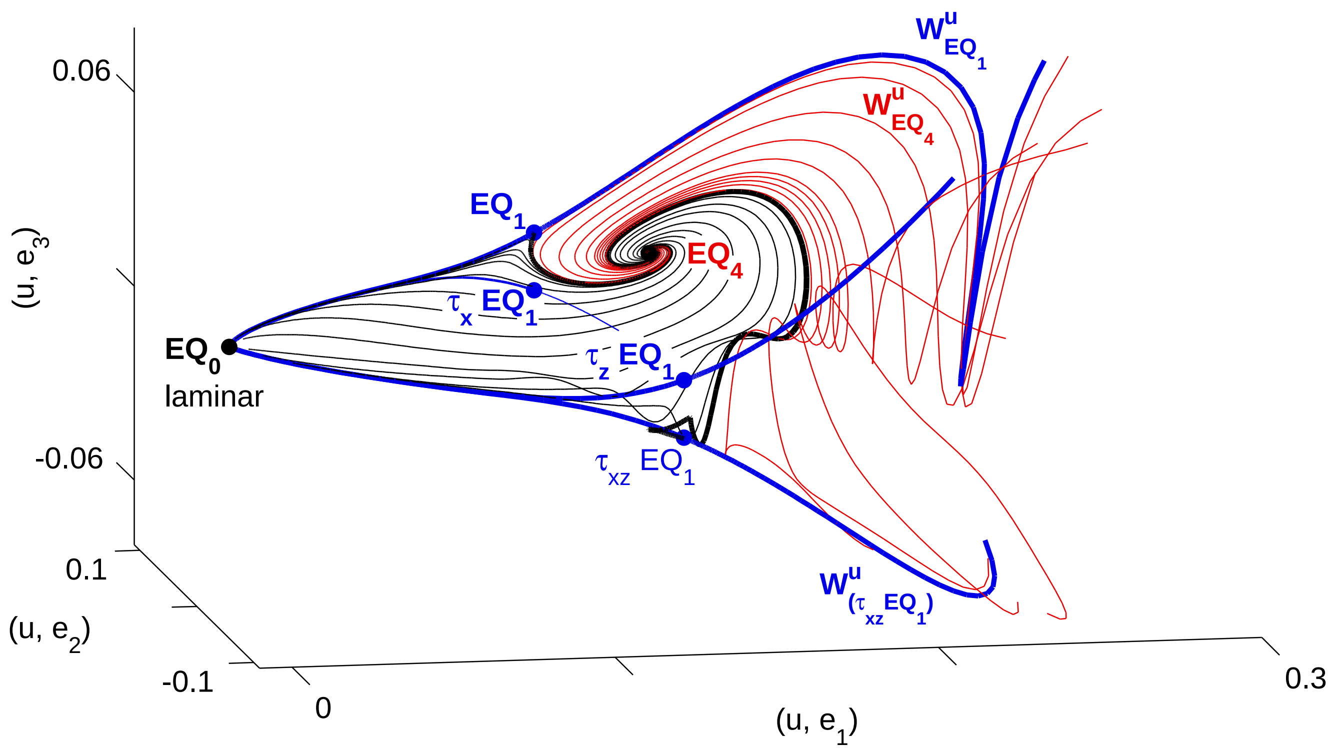


Equilibria


EQ5, lower branch
0.4
0
−0.4
−0.04
0
0.05
0.1
Re λ
Im λ

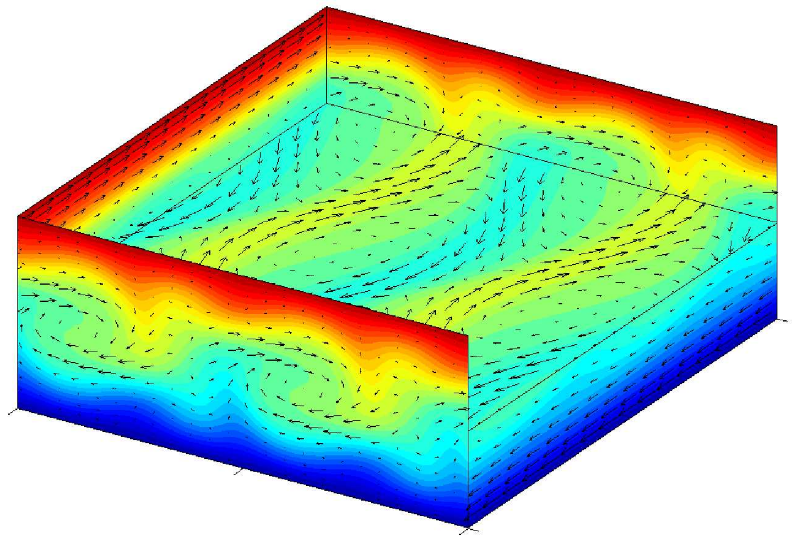

EQ6, upper branch
0.4
0
−0.4
−0.04
0
0.05
0.1
Re λ
Im λ

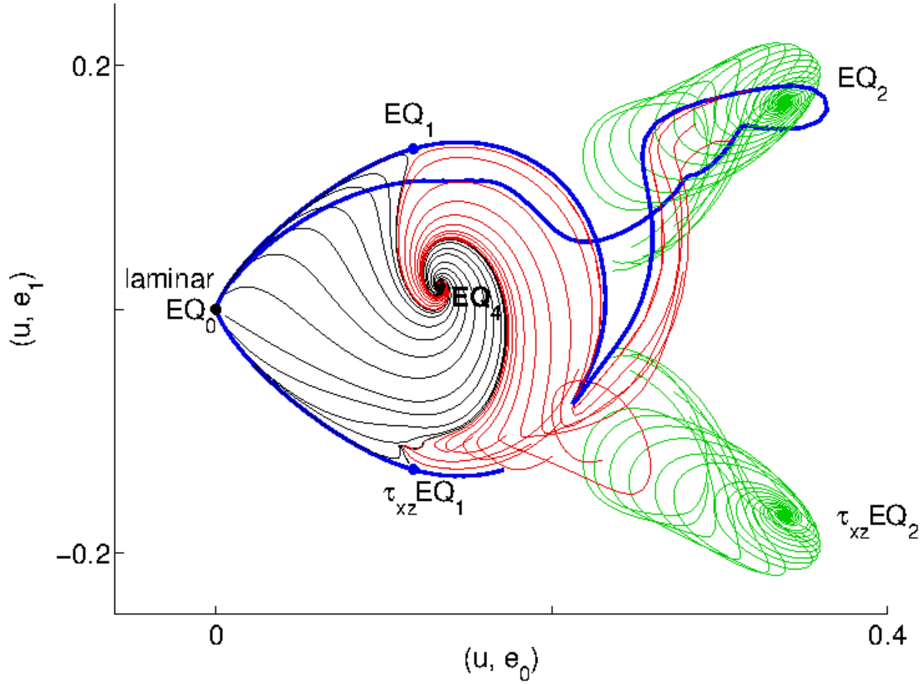
Equilibria organize dynamics: state space portraits



- 10^5-d DNS $\mathbf{u}$ projected onto 3d space spanned by a few EQBs
- Dots = equilibria
- Lines = unstable manifolds, heteroclinic connections, computed with DNS

Equilibria organize dynamics: heteroclinic connections





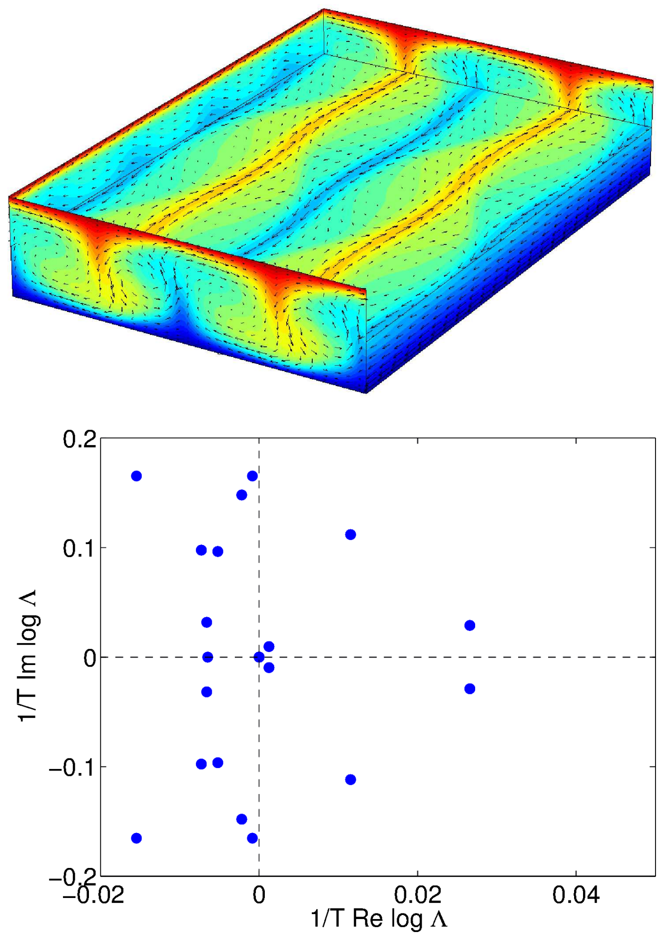
Animations:

- EQ$_4$ $\rightarrow$ EQ$_1$ heteroclinic connection: [3d movie] [x-average movie]
- EQ$_4$ $\rightarrow$ τ_{xz}EQ$_1$ heteroclinic connection: [3d movie] [x-average movie]
- [movie of transient turbulence]

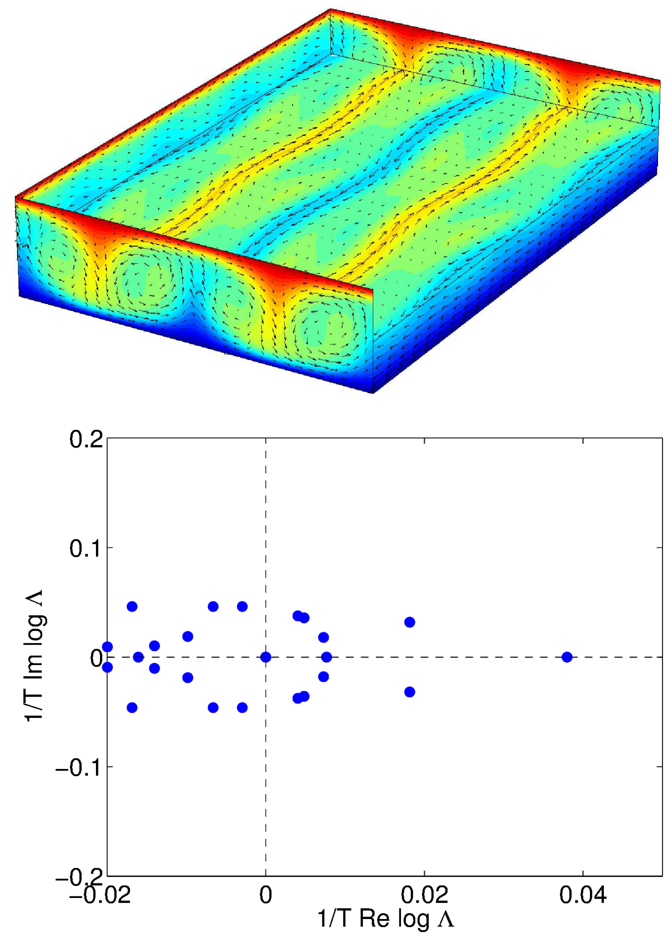
Halcrow, Gibson, Cvitanović, Viswanath, (2009) JFM 621

Periodic orbits

$T = 19.02$



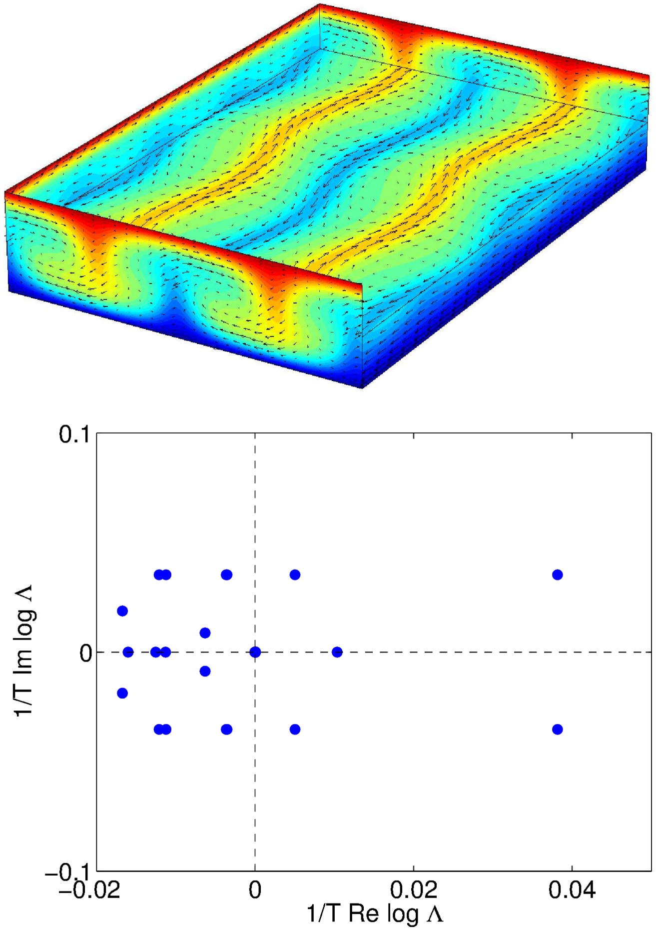
$T = 68.07$



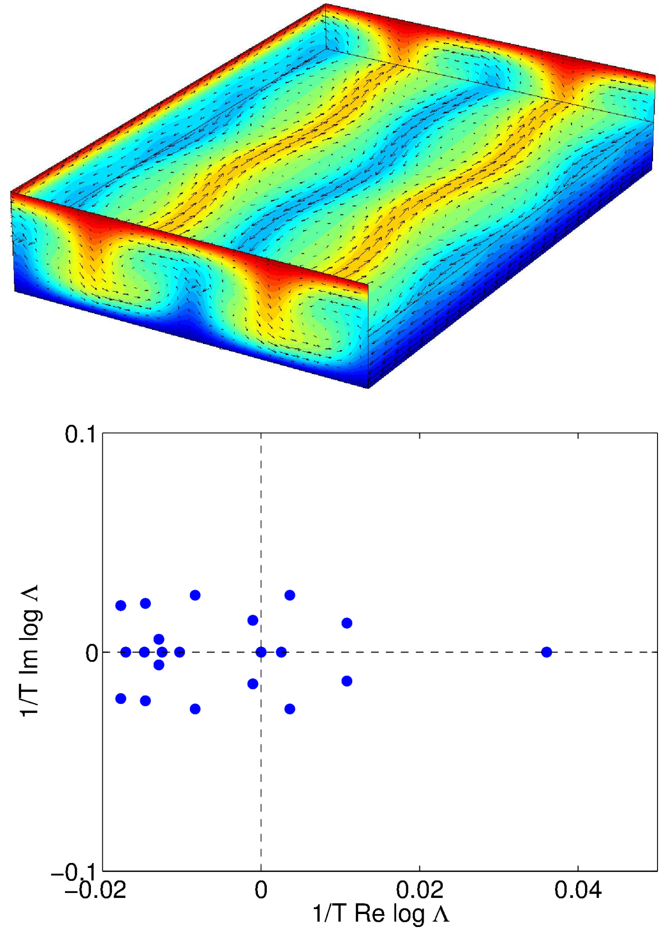
[movie of turbulent flow]

Periodic orbits

$T = 88.90$

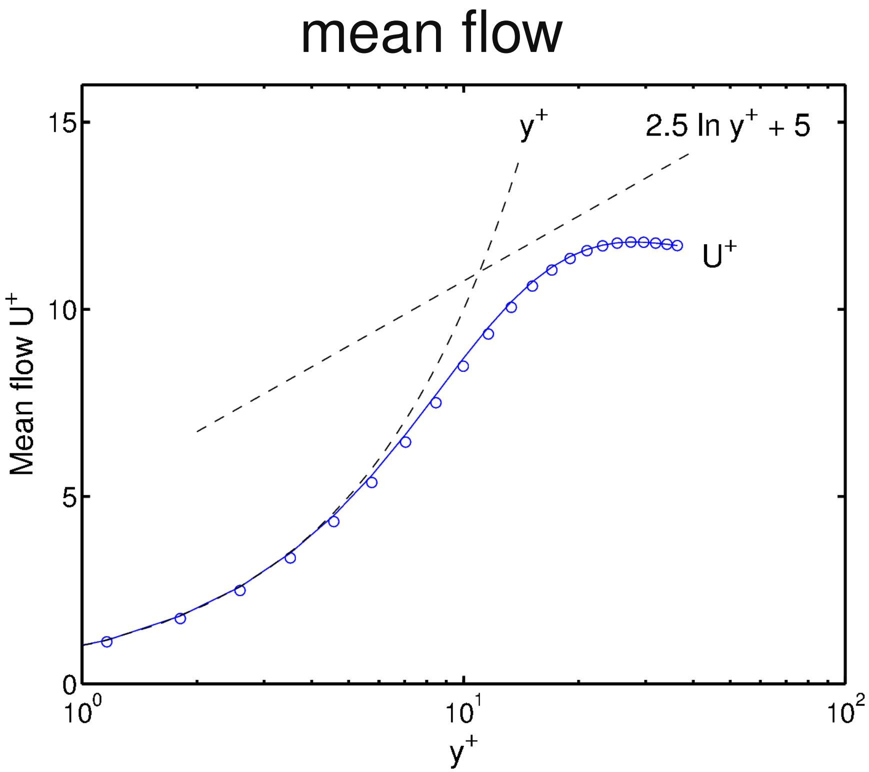


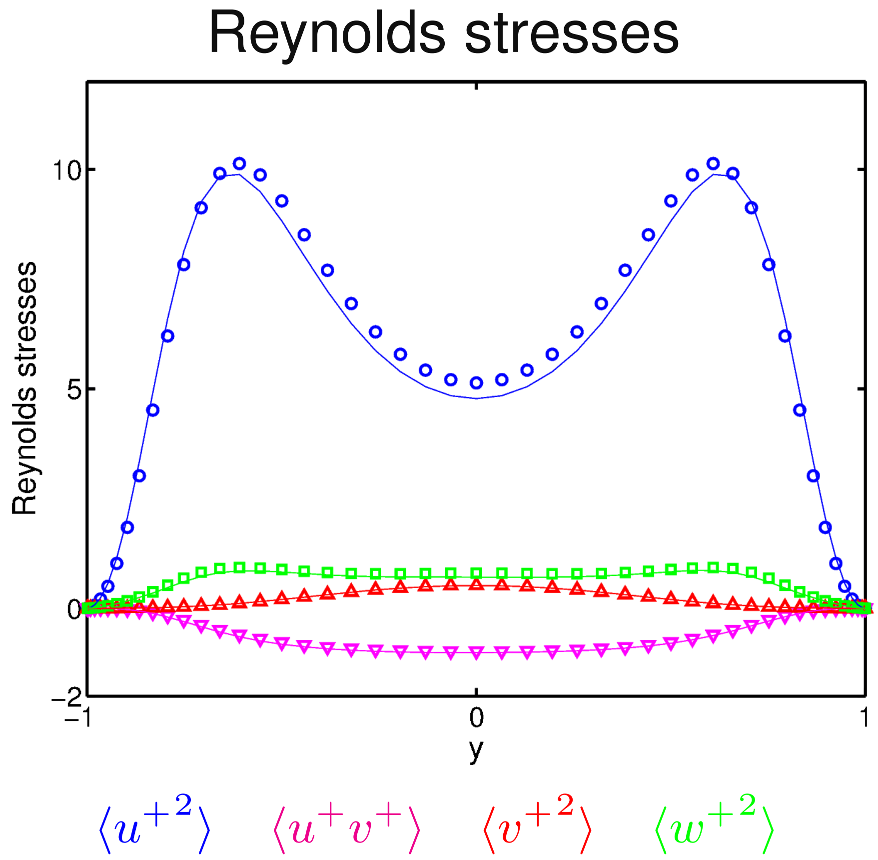
$T = 121.4$



[movie of turbulent flow]

Periodic orbits replicate statistics

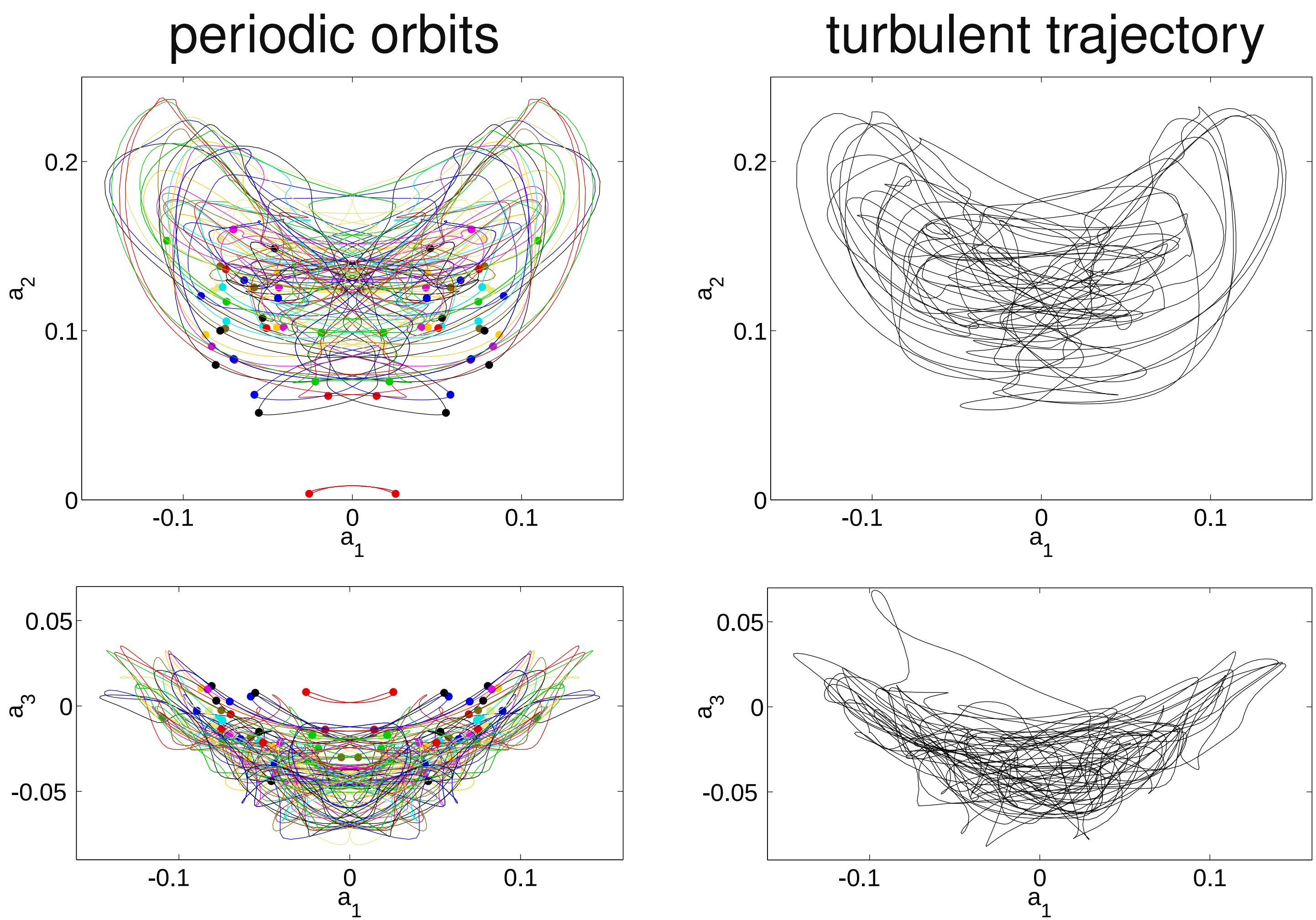




Turbulent flow (lines) versus $T = 121$ periodic orbit (symbols), $Re = 400$

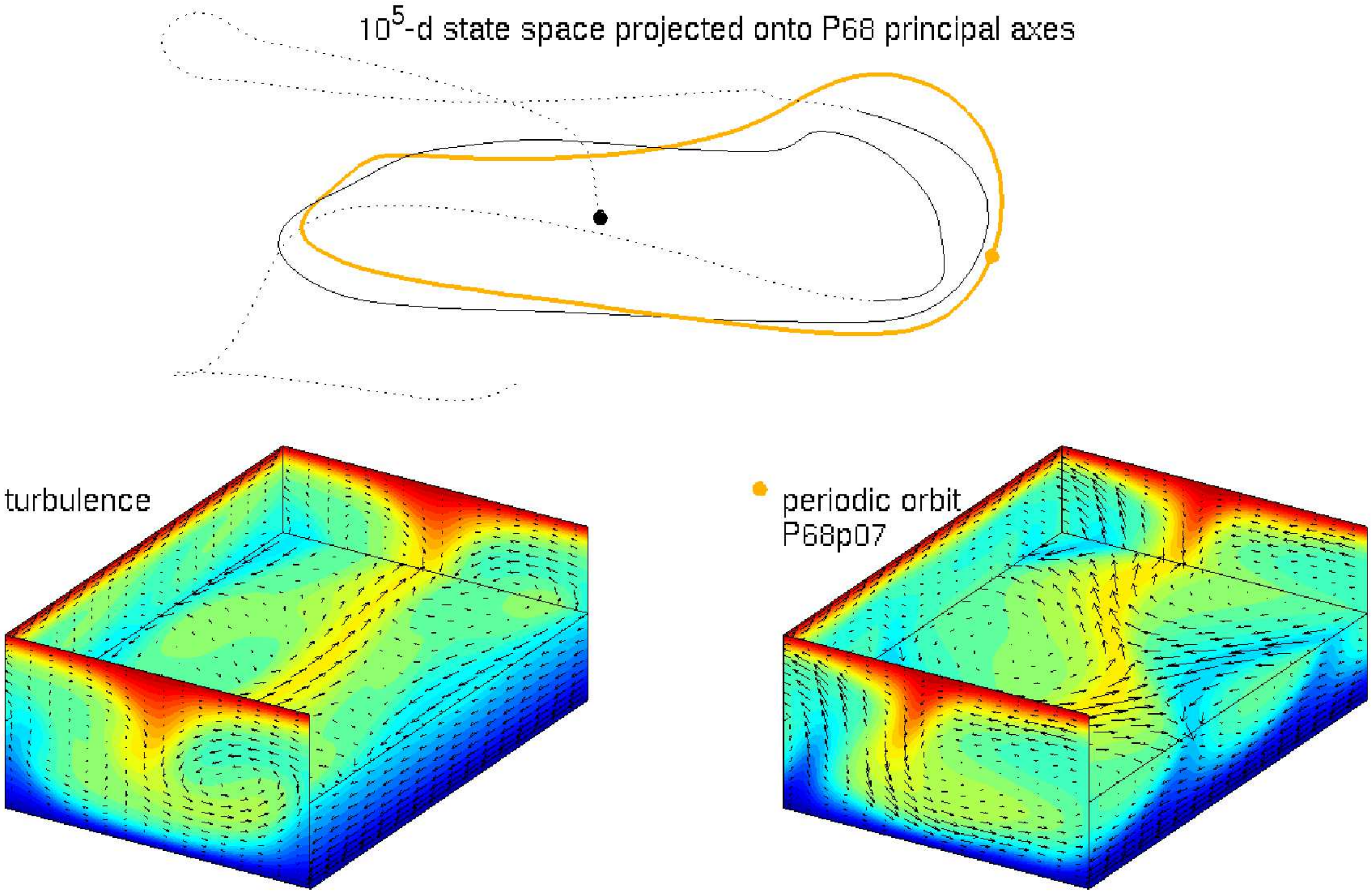
Typical orbits have mean flow to 1% and Reynolds stresses to 5-10%.

Ensemble of periodic orbits versus invariant measure

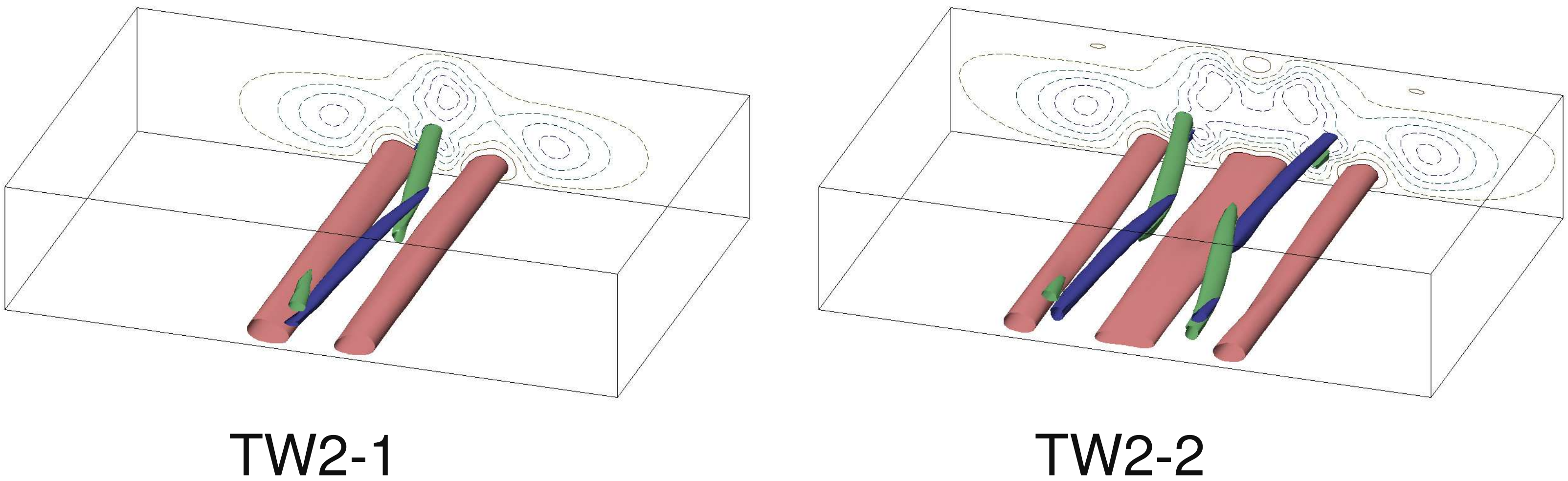


10^5-d DNS states $\mathbf{u}$ projected onto principal axes of a periodic orbit.

Turbulence shadowing a periodic orbit

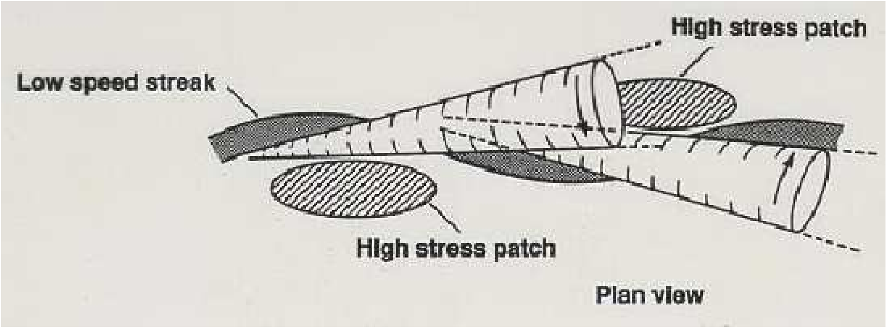


Spatially localized traveling waves of channel flow

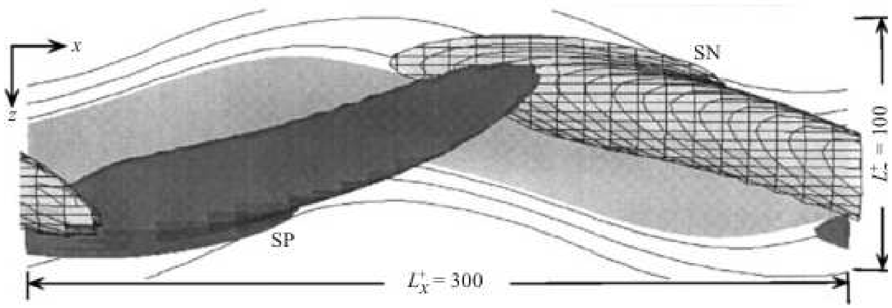


- concentrated, alternating, tilted, near-wall streamwise rolls
- centered over low-speed streaks, flanked by high-speed streaks
- large streamwise velocity deficit in core, relative to laminar

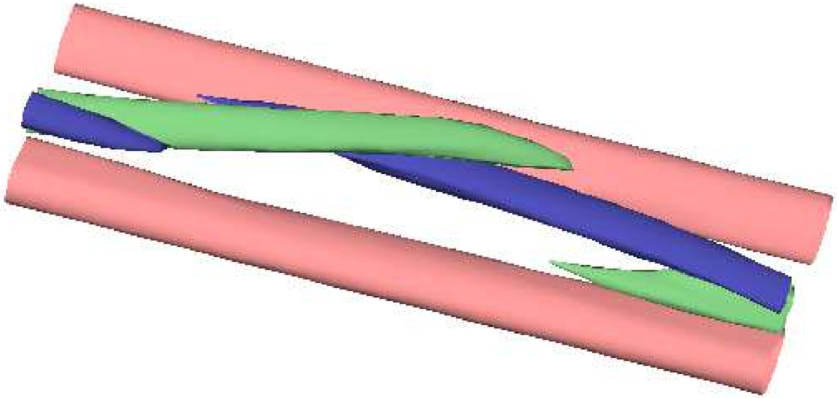
Comparison to sinuous boundary-layer structures



Stretch (1990)
educed from DNS data

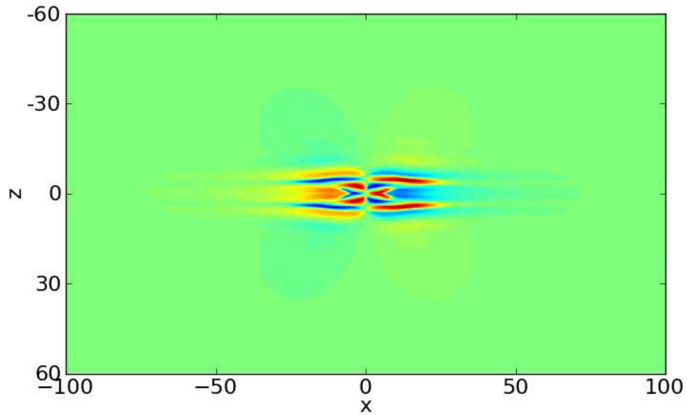


Schoppa & Hussain (2002)
transient growth mode

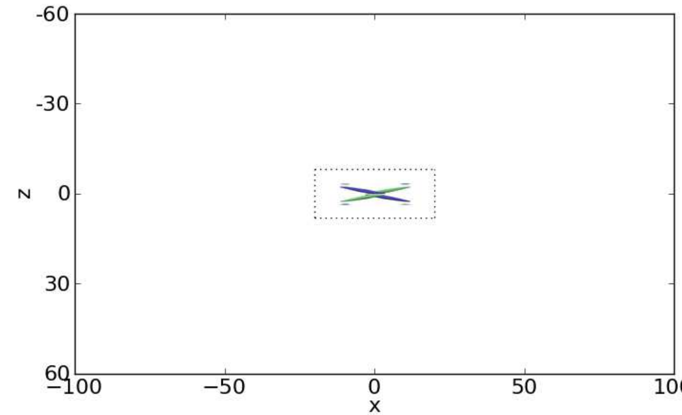


TW2-1: exact traveling wave of channel flow
same orientation of swirling, wall-unit length scales

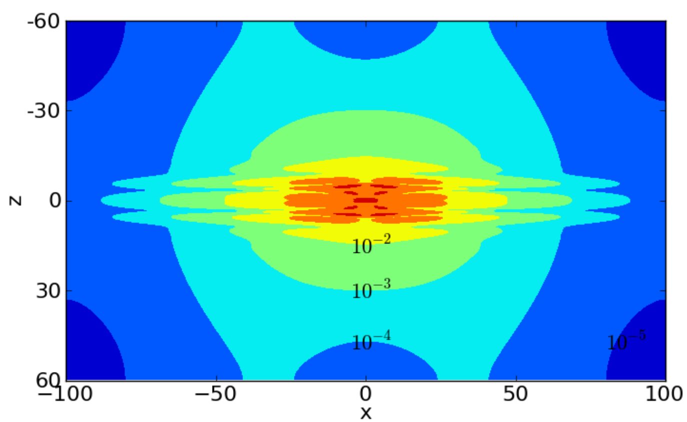
Doubly-local equilibrium of plane Couette



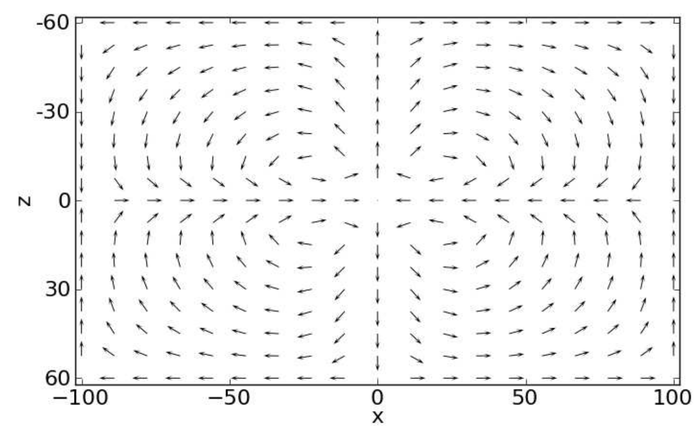
midplane streamwise velocity



swirling strength



y-avg energy



normalized y-avg (u,w) flow

small nonlaminar spot decaying exponentially to laminar flow

Bibliography

PCF = plane Couette flow, PPF = plane Poiseuille or channel flow
ASBL = asymptotic suction boundary layer

- Nagata 1990: equilibrium solution of PCF
- Waleffe 1995-2003: self-sustaining process, traveling waves of PPF
- Kawahara, Kida 2001: 2 periodic orbits in PCF
- Faisst, Eckhardt 2003: traveling waves in pipe flow
- van Veen, Kida, Kawhara 2006: periodic orbits of isotropic turbulence
- Viswanath 2007: Newton-Krylov-hookstep algorithm, 5 periodic orbits PCF
- Schneider, Eckhardt, and Marinc 2010: spanwise-localized PCF solutions
- Schneider, Gibson, Burke 2010: homoclinic snaking of PCF solutions
- Khapko, Kreilos, Eckhardt et al. 2013 periodic orbits of ASBL
- Willis, Cvitanovic, Avila 2013: symmetry reduction for solutions of pipe flow
- Gibson, Brand 2014, spanwise- and wall-localized traveling waves of PPF and doubly-localized equilibrium of PCF

Kawahara, Uhlman, van Veen, Annual Review Fluid Mech. 2012

Key conclusions

- Exact coherent structures = invariant solutions of Navier-Stokes.
- Computed as exact solutions of DNS.
- Replicate observed flow features: roll/streak structures, bursting, mean flow, Reynolds stresses.
- Low-d instabilities, dynamics wanders within low-d unstable manifolds.
- Observed coherent structures = close passes to exact coherent structures.
- **Provides precise, model-free, low-d approach to transitional turbulence.**

Questions and directions

- High Reynolds numbers
- Multiple-scale solutions
- Extended flows, localized solutions
- Open flows, e.g. boundary layer
- Dynamical models based on low-d linearization about orbits
- Statistics via periodic orbit theory

Thanks to collaborators:

Predrag Cvitanovic, Jonathan Halcrow, Divikar Viswanath,

Tobias Schneider, Evan Brand.