Dynamics and Data

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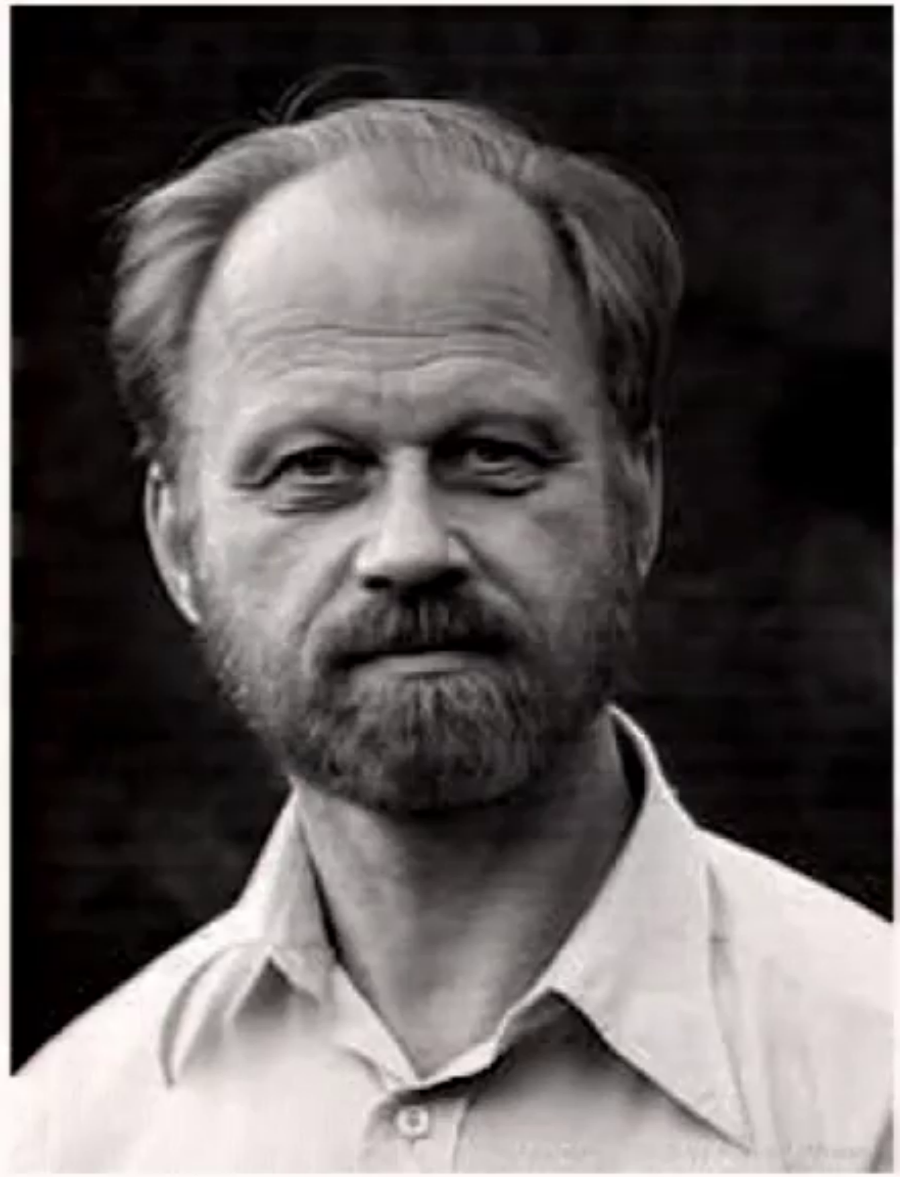
SIAM Jürgen Moser Lecture
May, 2015

Jürgen Moser

Mentor early in my career

- IAS 1971-72
- Editor of Inventiones
- CIME, Bressanone
- Courant 1978



Dynamical patterns – Principles

- Synergy of theory, experiment and computation
- “Simple” examples reveal general theory
- Genericity as a strategic viewpoint

Outline

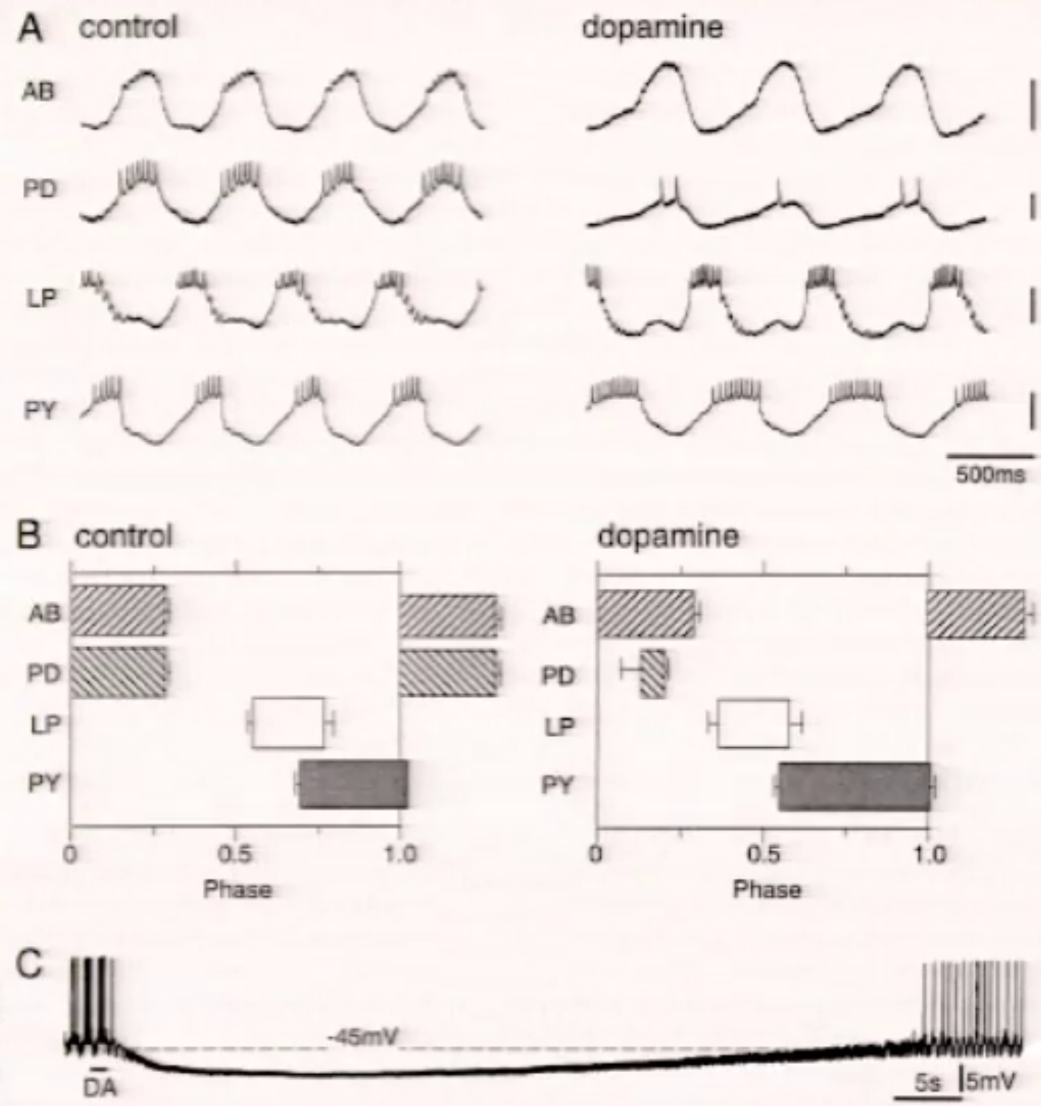
1. Multiple time scales: neurons
2. Mixed mode oscillations: chemical reactors
3. Periodic orbits: locomotion

Future: power grids?

Pyloric Circuit of Stomatogastric Ganglion

Neural network of 14 neurons in lobster

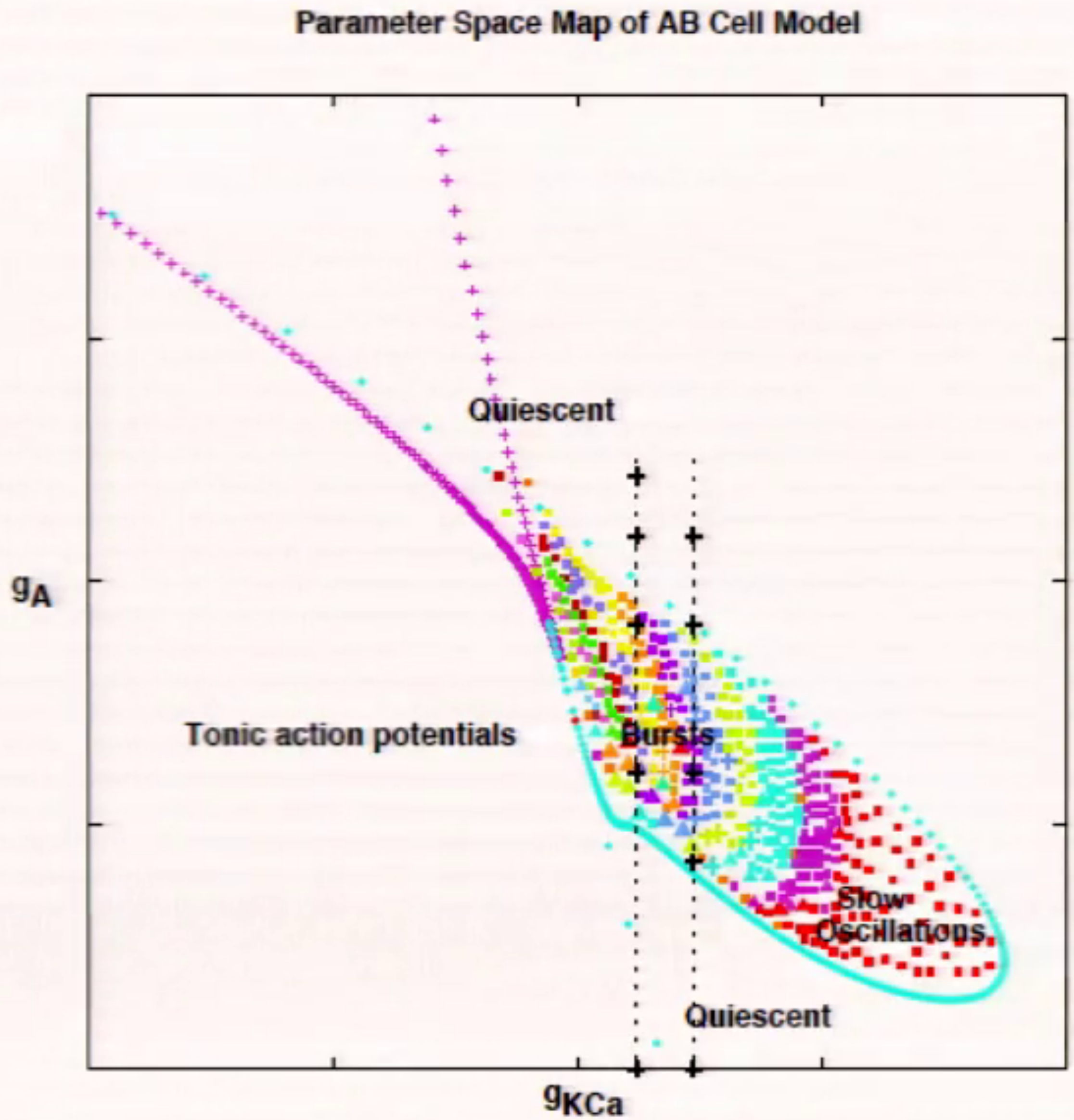
- Action potentials drive motor activity
- Several network rhythms
- Hodgkin-Huxley type models of neurons
- Voltage clamp measurements
- Experiments test neuromodulation



Harris-Warrick laboratory

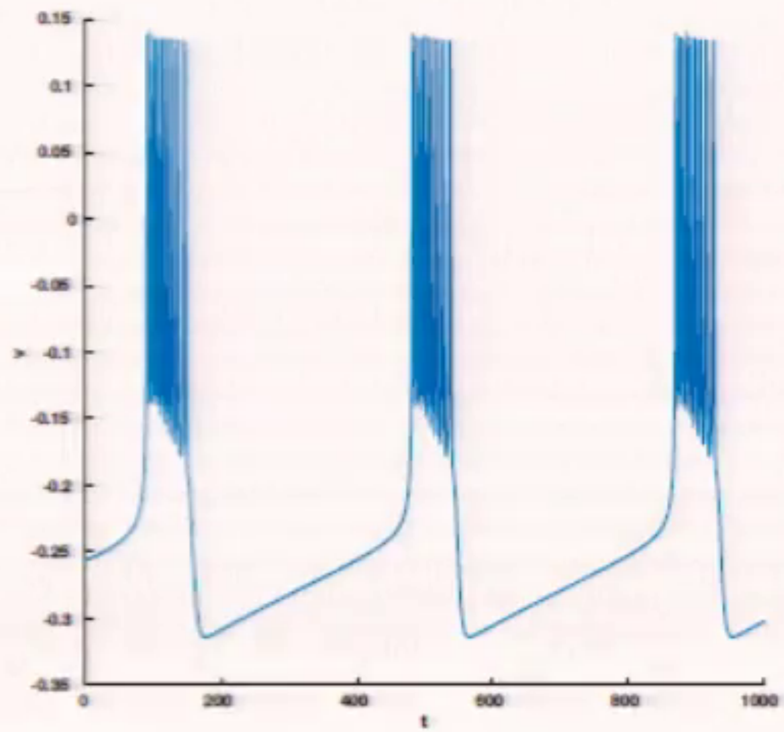
Multi-parameter Study of AB Cell

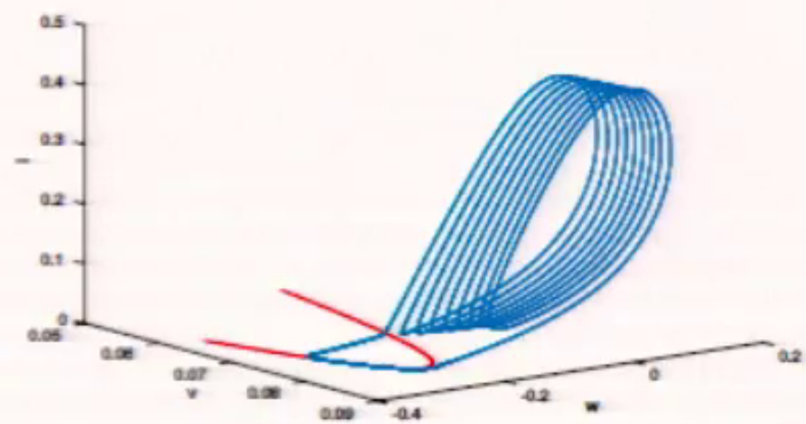
- 5 dimensional vector field
- 20+ parameters
- Bifurcation curves via continuation
- Measured blockade of A current
- Sensitivity to g_{KCa}
- New algorithm for double Hopf bifurcation



Bursting

- Rinzel: multiple time scales
- Qualitative classification via bifurcations
- Interspike intervals: homoclinic vs SNIC
- Quantitative classification: duty cycle
- Automatic differentiation: sensitivities to parameters
- Challenge: data fitting





Geometric Singular Perturbation Theory

Three approaches to dynamics with multiple time scales

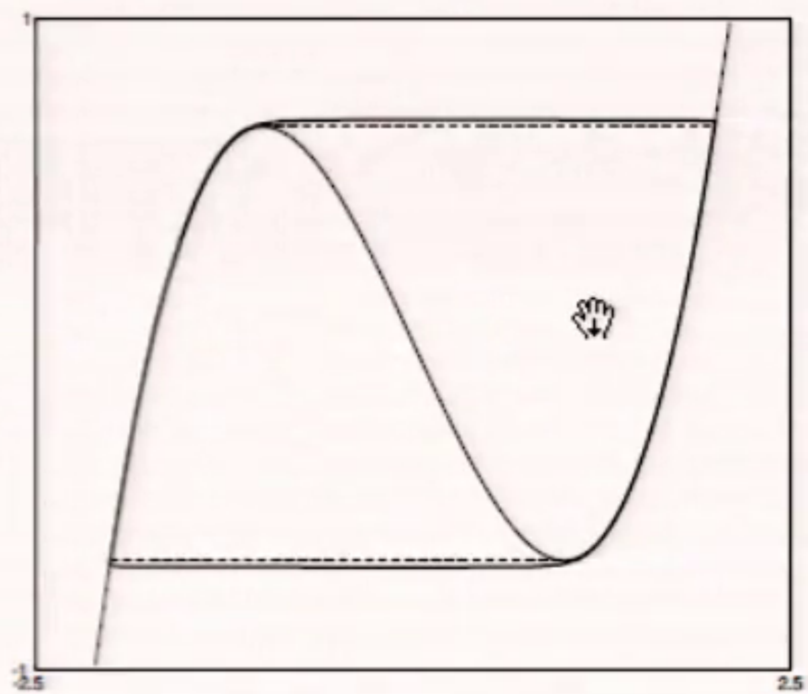
- Asymptotic analysis (Russia 1940s)
- Non-standard analysis (Strasbourg 1970s)
- GSPT (Fenichel 1970s)

Slow-fast vector fields

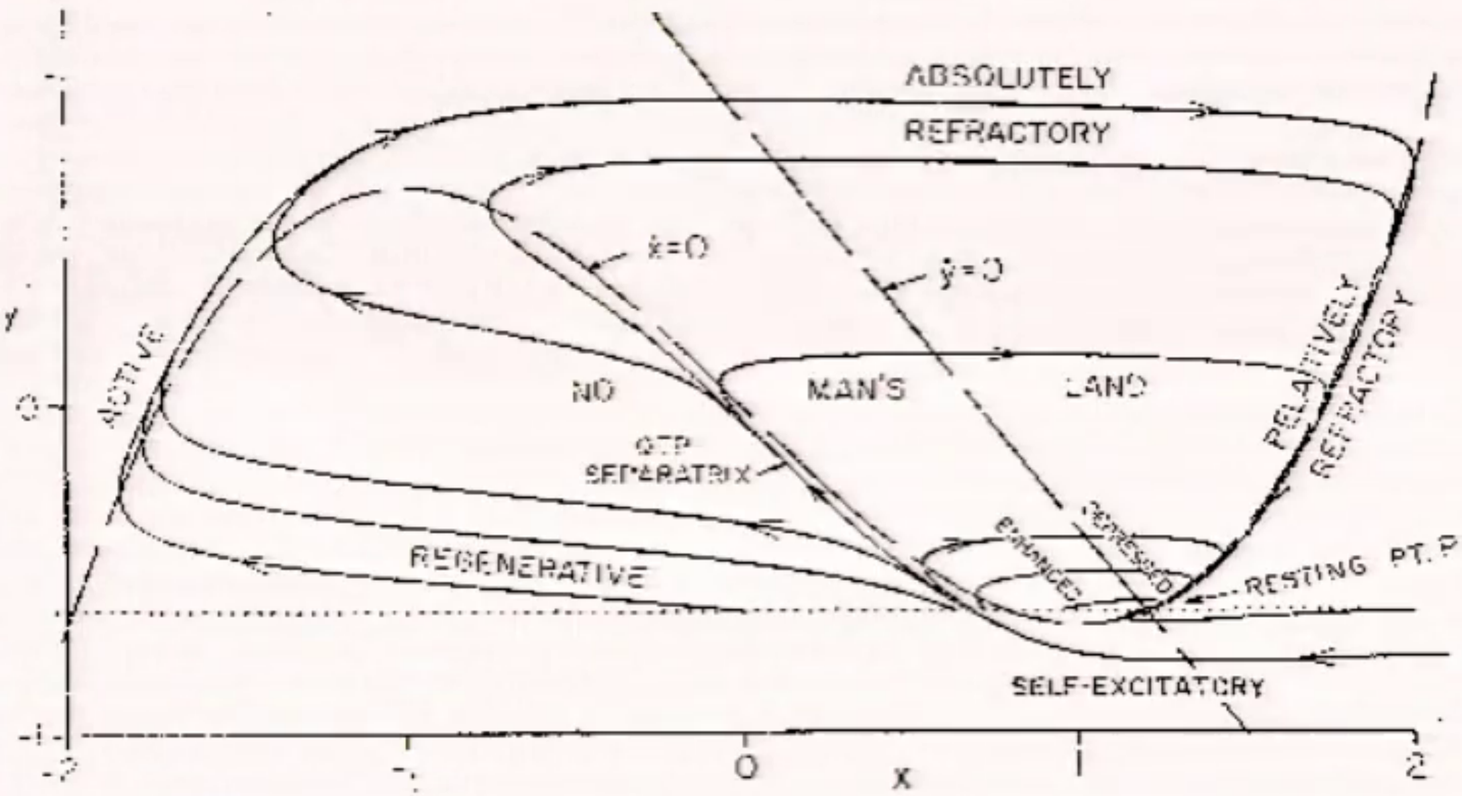
$$\begin{aligned} \varepsilon\dot{x} &= f(x,y) \qquad x \in R^m \\ \dot{y} &= g(x,y) \qquad y \in R^n \end{aligned}$$

Van der Pol equation

$$\begin{aligned} \varepsilon\dot{x} &= y - x^3 + x \\ \dot{y} &= -x \end{aligned}$$



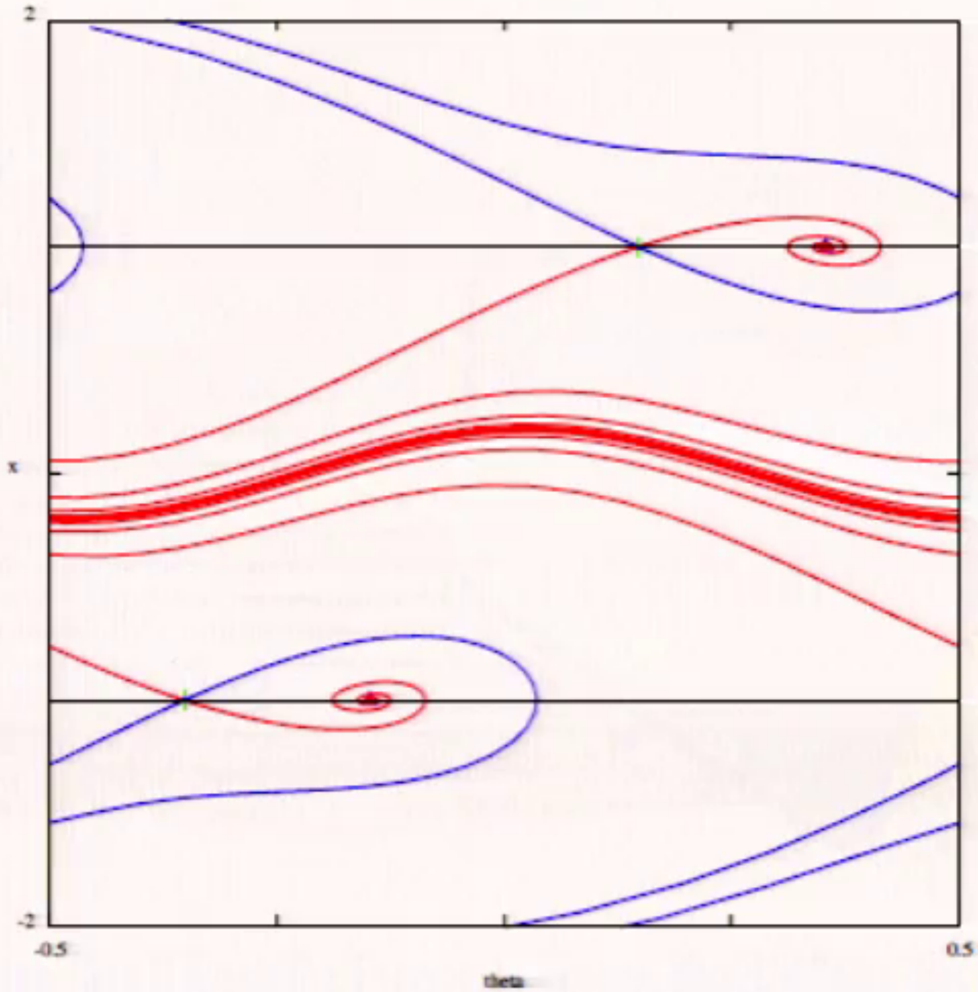
FitzHugh 1961: No Man's Land



$$\varepsilon \dot{x} = c(y + x - \frac{x^3}{3})$$

$$\dot{y} = -(x - a + by)/c$$

Desingularized Reduced Forced van der Pol System

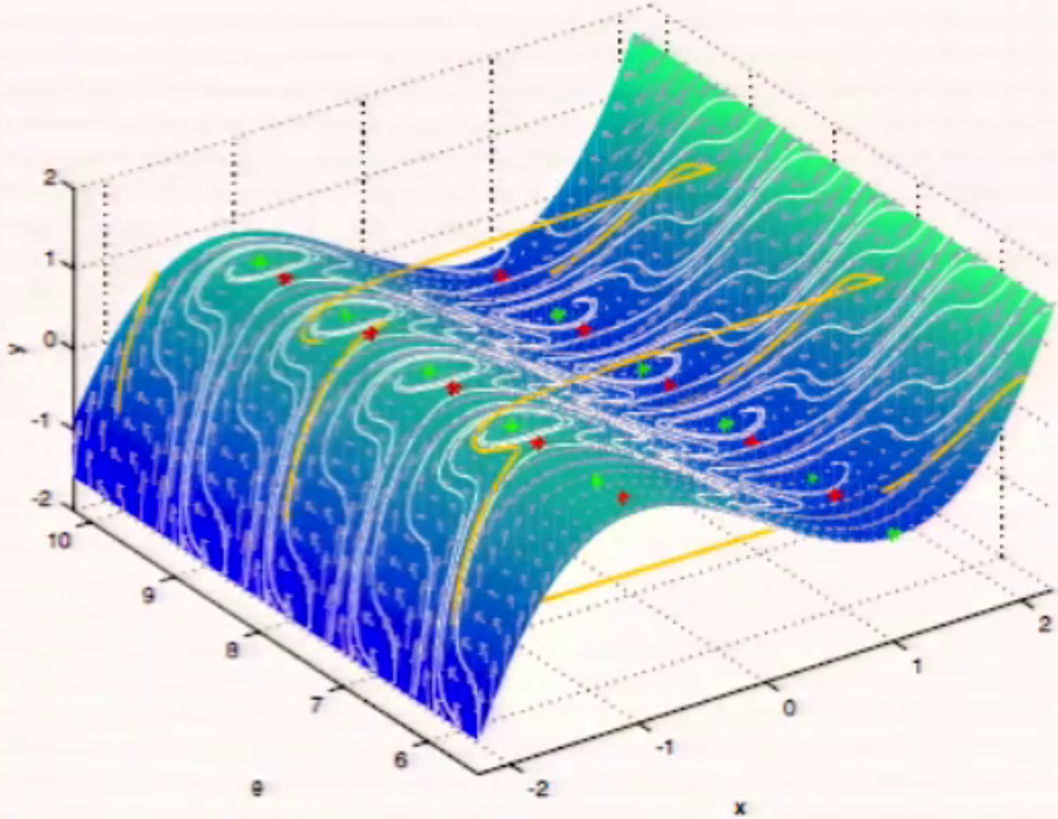


$a = 1.5 \ \omega = 1$

Forced Van der Pol Equation

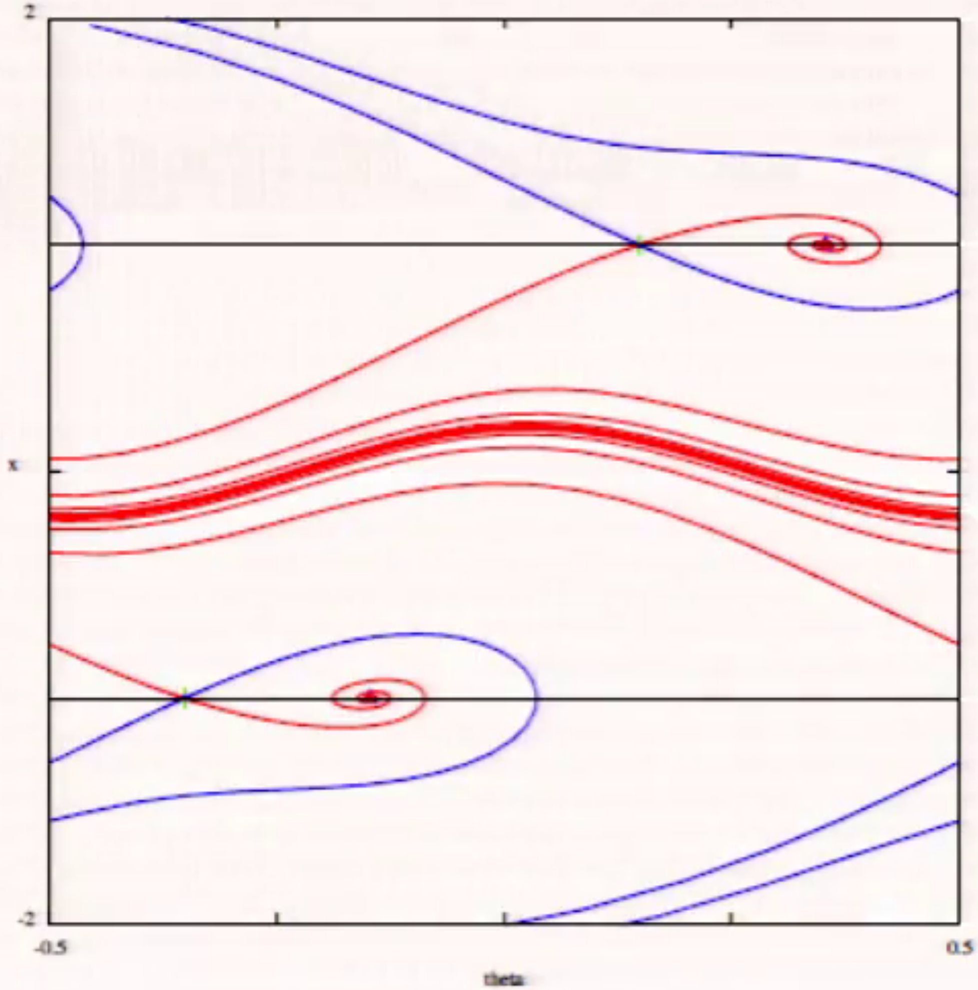
Littlewood 1957: first analysis of chaos in dissipative system

$$
\begin{aligned}
\varepsilon \dot{x} &= y + x - \frac{x^3}{3} \\
\dot{y} &= -x + a\sin(2\pi\theta) \\
\dot{\theta} &= \omega
\end{aligned}
$$



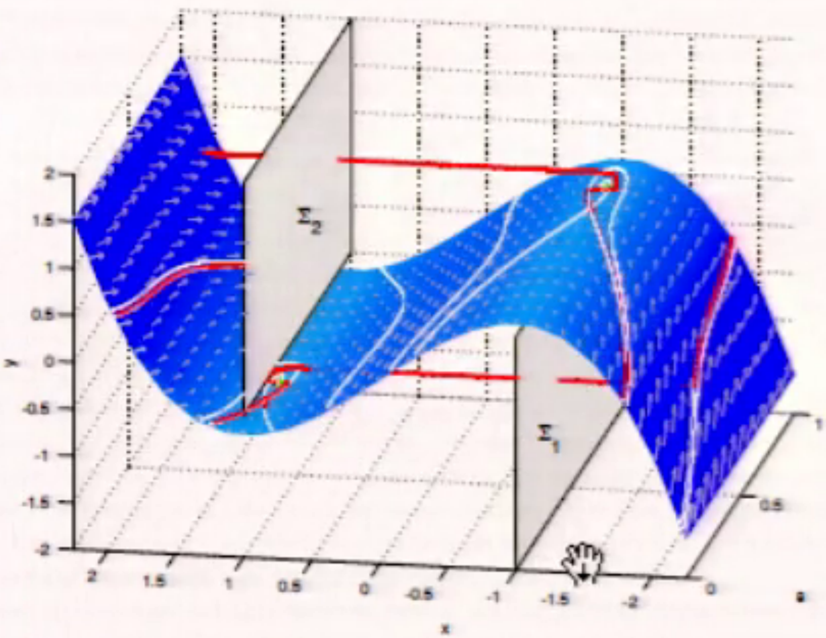
- Inspiration for Smale horseshoe, but details poorly assimilated
- Haiduc 2009 proves that system is Axiom A and structurally stable

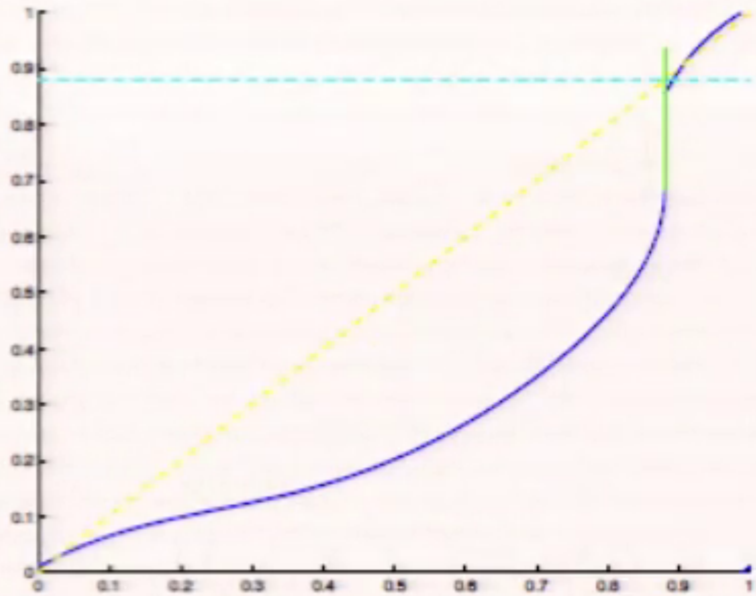
Desingularized Reduced Forced van der Pol System



$a = 1.5 \ \omega = 1$

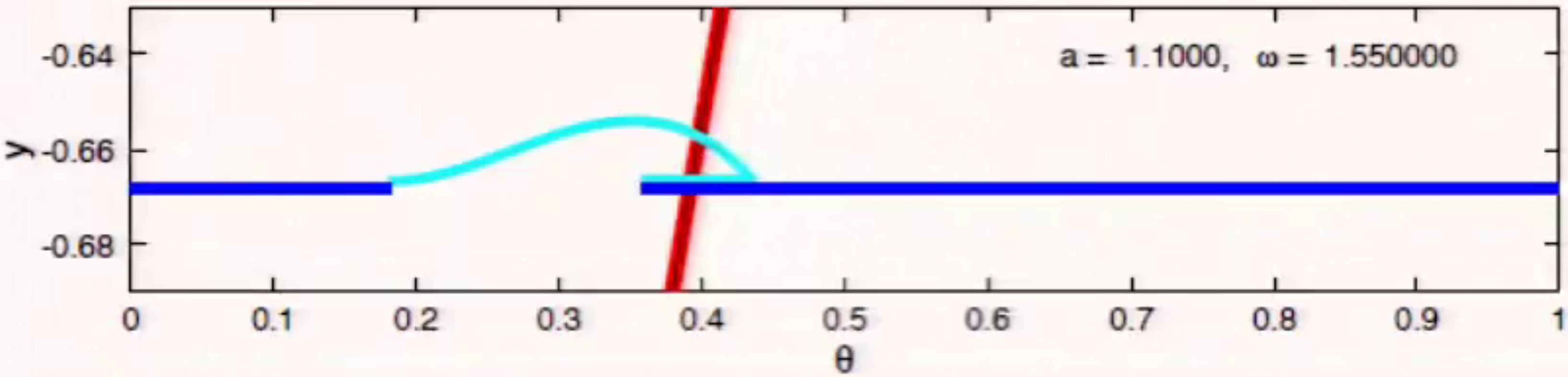
Forced van der Pol Half Return Map



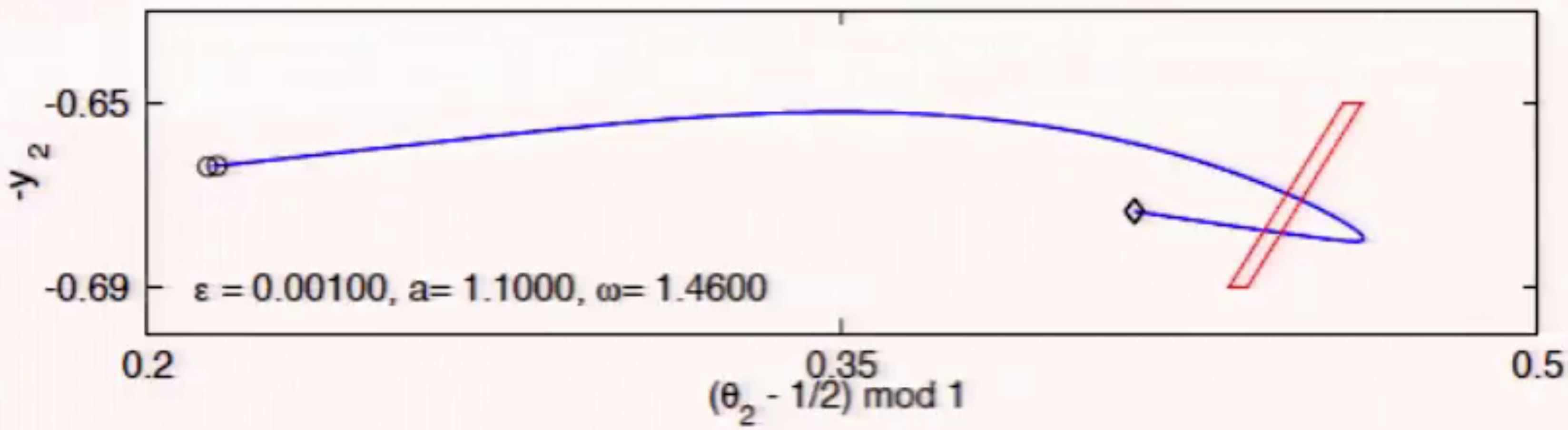


- Follow trajectories from Σ_1 to Σ_2
- Include jumps from points on canards
- Canards produce green vertical segments in return map

Forced van der Pol Horseshoe



Singular half return map P: $(a, \omega) = (1.1, 1.55)$



Computation of P with AUTO: $(a, \omega, \varepsilon) = (1.1, 1.46, 0.001)$

Mixed Mode Oscillations in BZ Reaction

Hudson, Hart, Marinko (1979) J. Chem. Phys. 71:1601-1606

Homogeneous stirred tank reactor: different flow rates

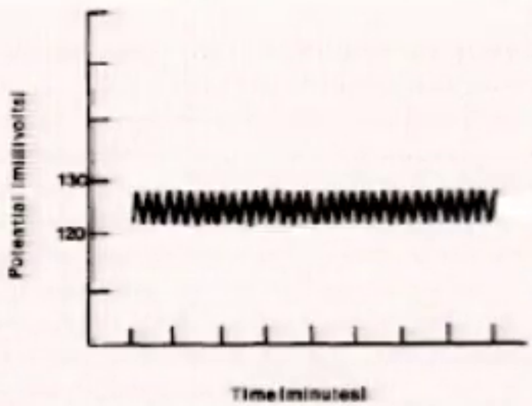


FIG. 11. Recording from bromide ion electrode; T = 25 °C; flow rate = 5.42 ml/min; Ce^{+3} catalyst.

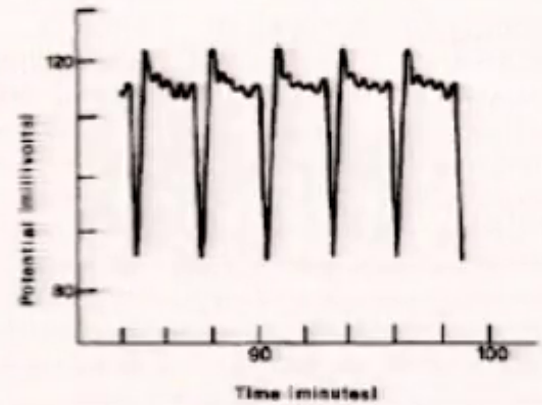


FIG. 9. Recording from bromide ion electrode; T = 25 °C; flow rate = 4.81 ml/min; Ce^{+3} catalyst.

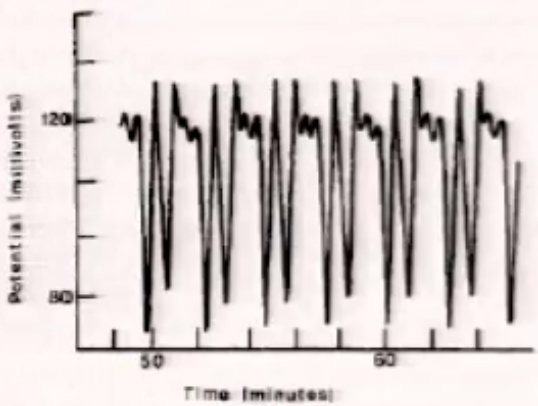


FIG. 12. Recording from bromide ion electrode; T = 25 °C; flow rate = 3.99 ml/min; Ce^{+3} catalyst.

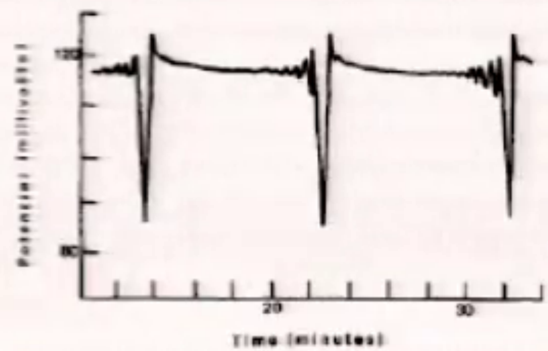
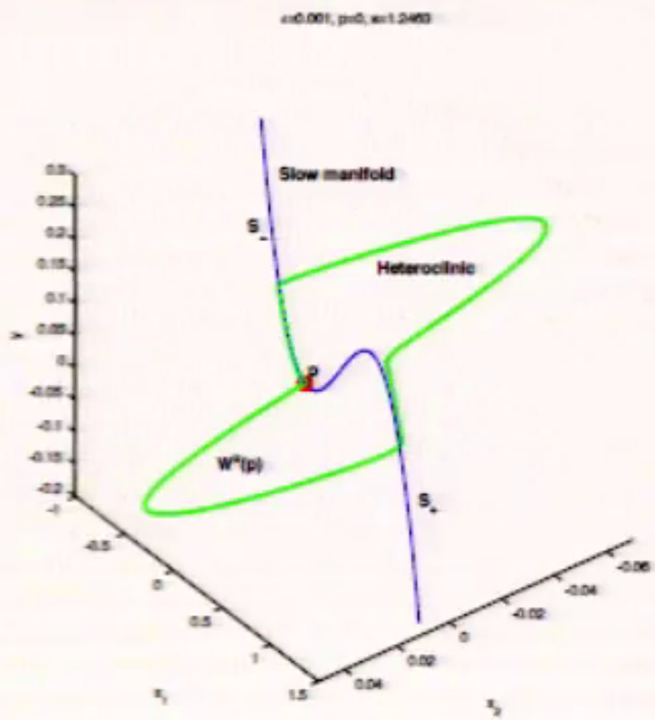


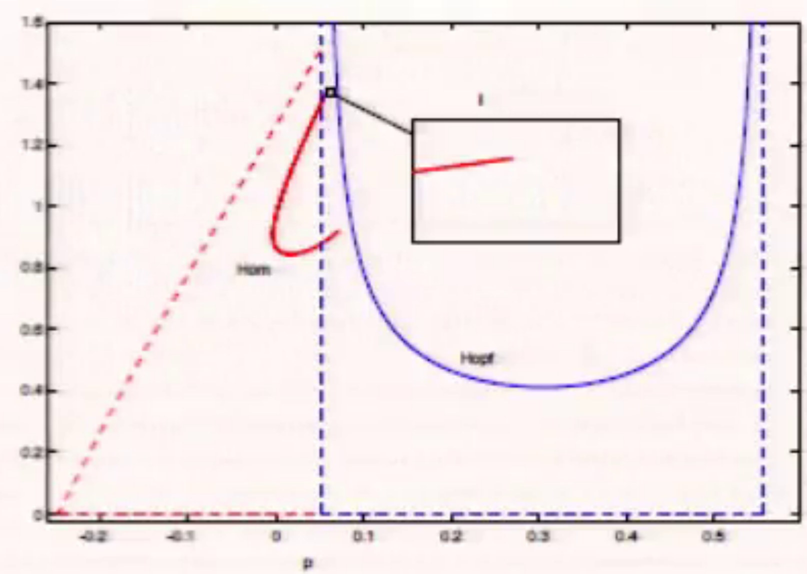
FIG. 10. Recording from bromide ion electrode; T = 25 °C; flow rate = 5.37 ml/min; Ce^{+3} catalyst.

FitzHugh-Nagumo Traveling Waves

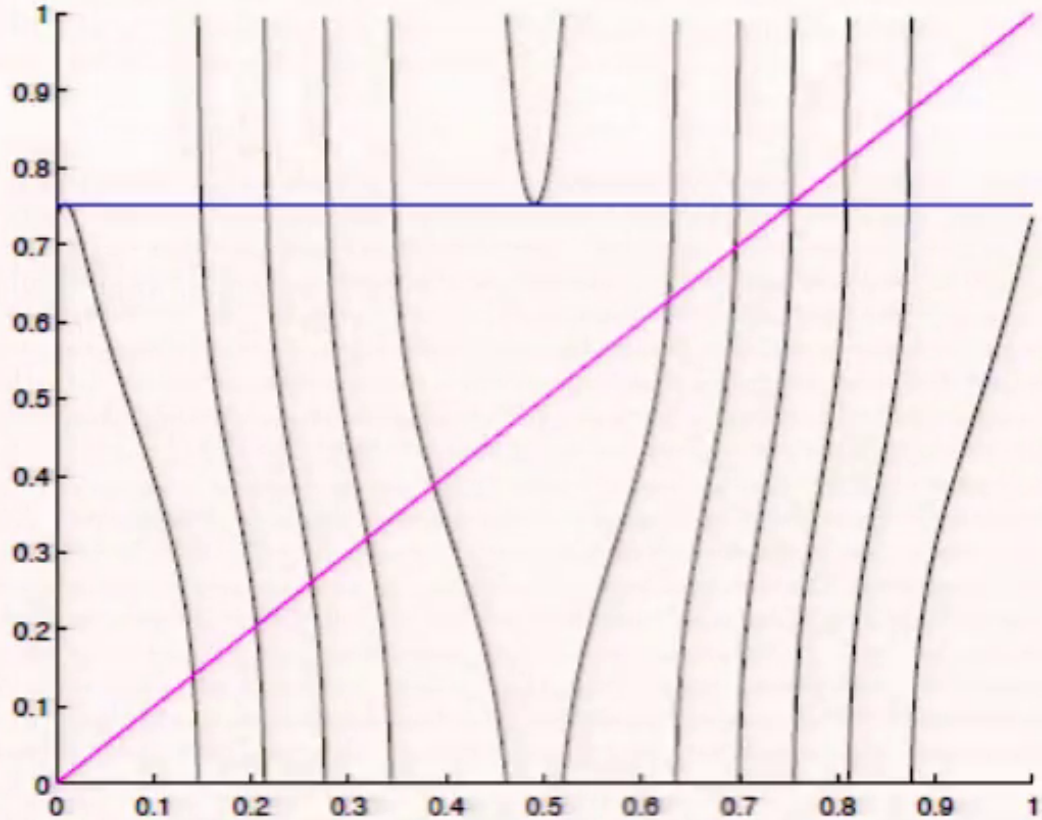
Analysis "easier" than numerics

- 1 slow and 2 fast variables
- Homoclinic orbits follow slow manifolds of saddle type
- Exchange Lemma
- Initial value solver cannot follow slow manifolds
- Homoclinic branch "ends" at tangency of two dimensional invariant manifolds





Chaotic Attractors in a Modified van-der Pol Equation



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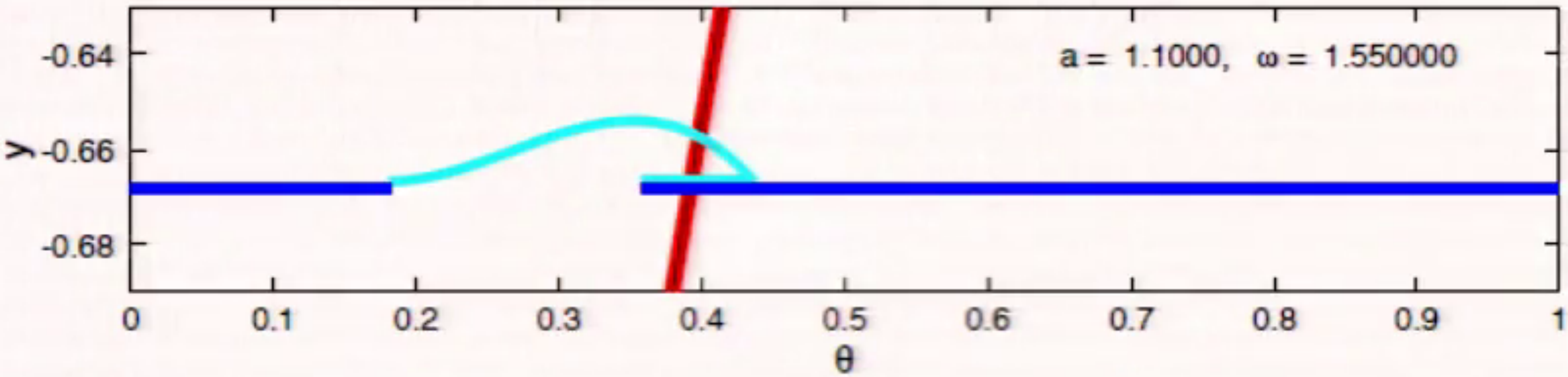
Guckenheimer, Wechselberger, Young (2006)

Forced van der Pol Horseshoe



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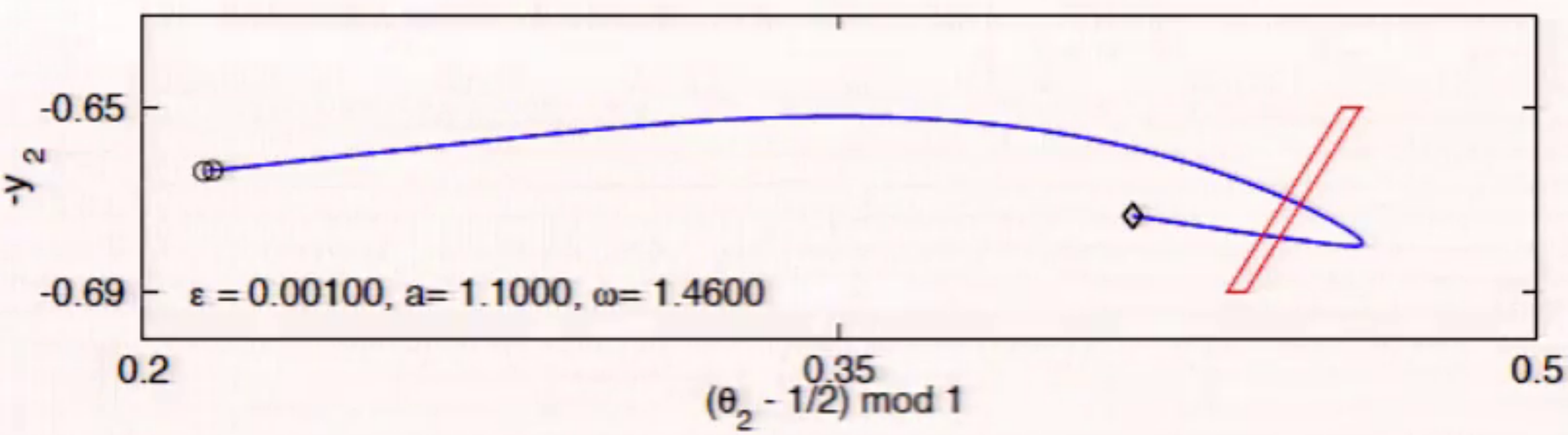

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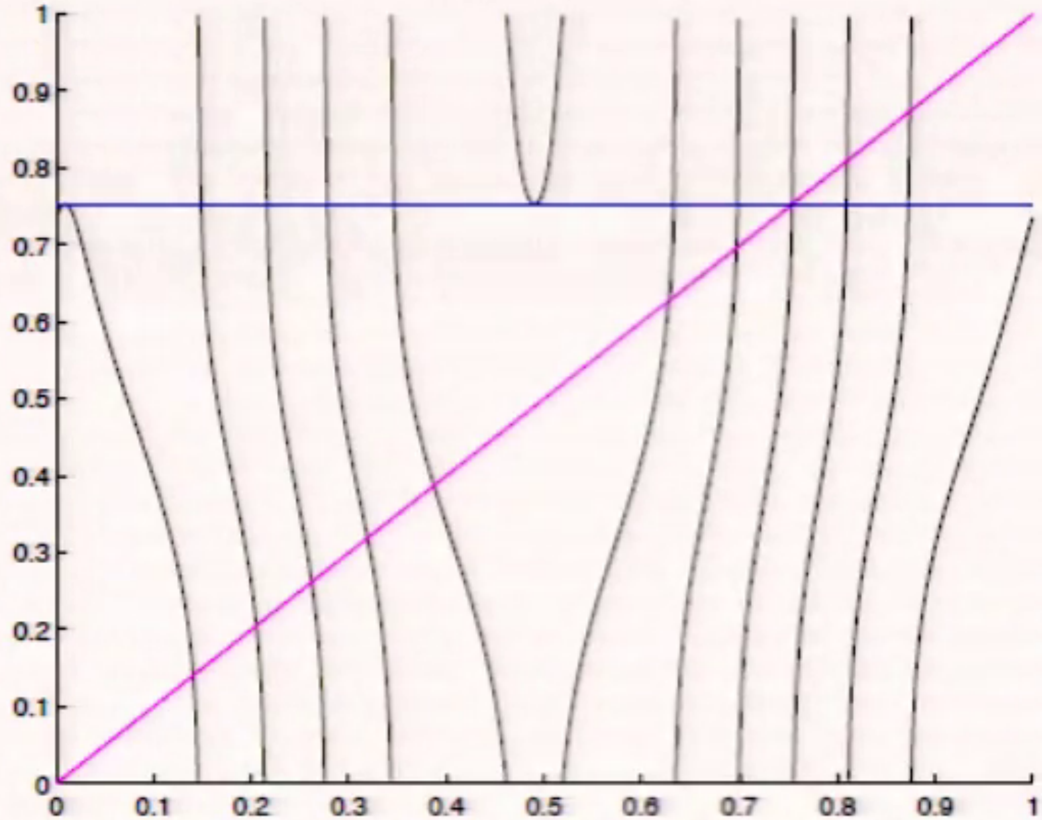

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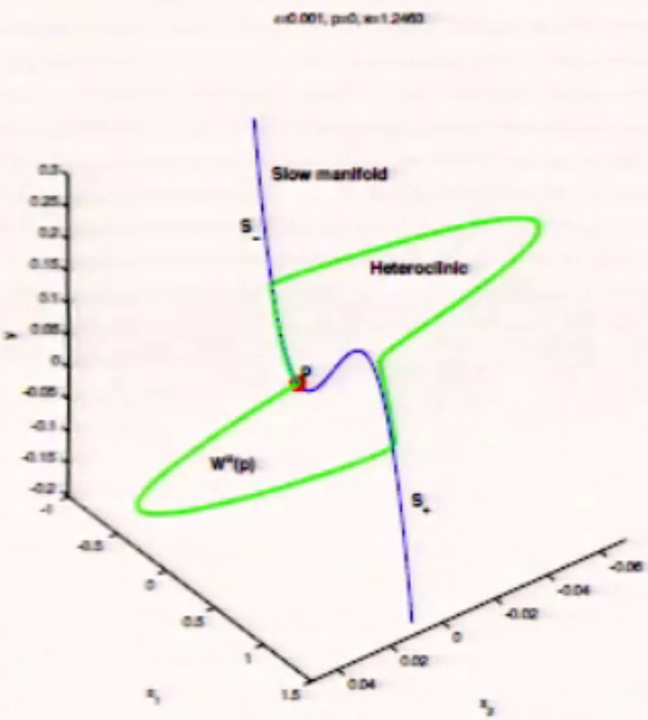
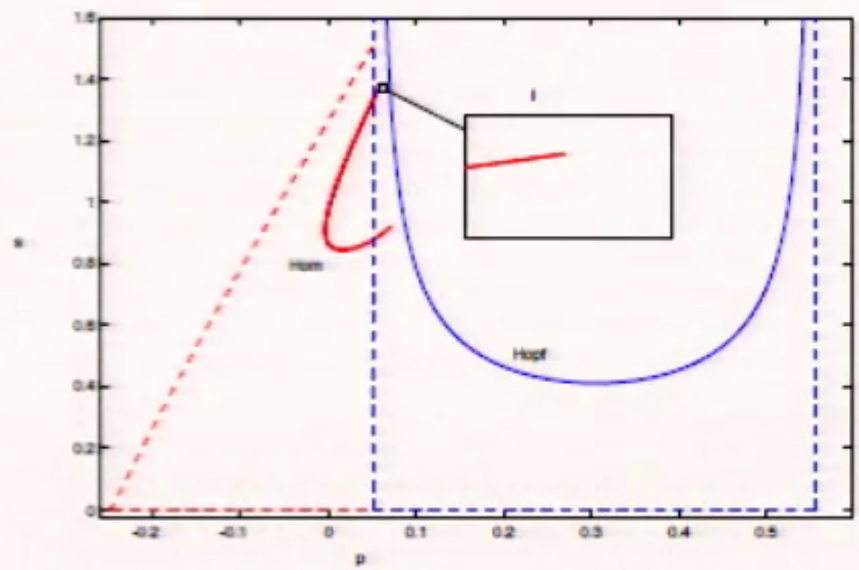
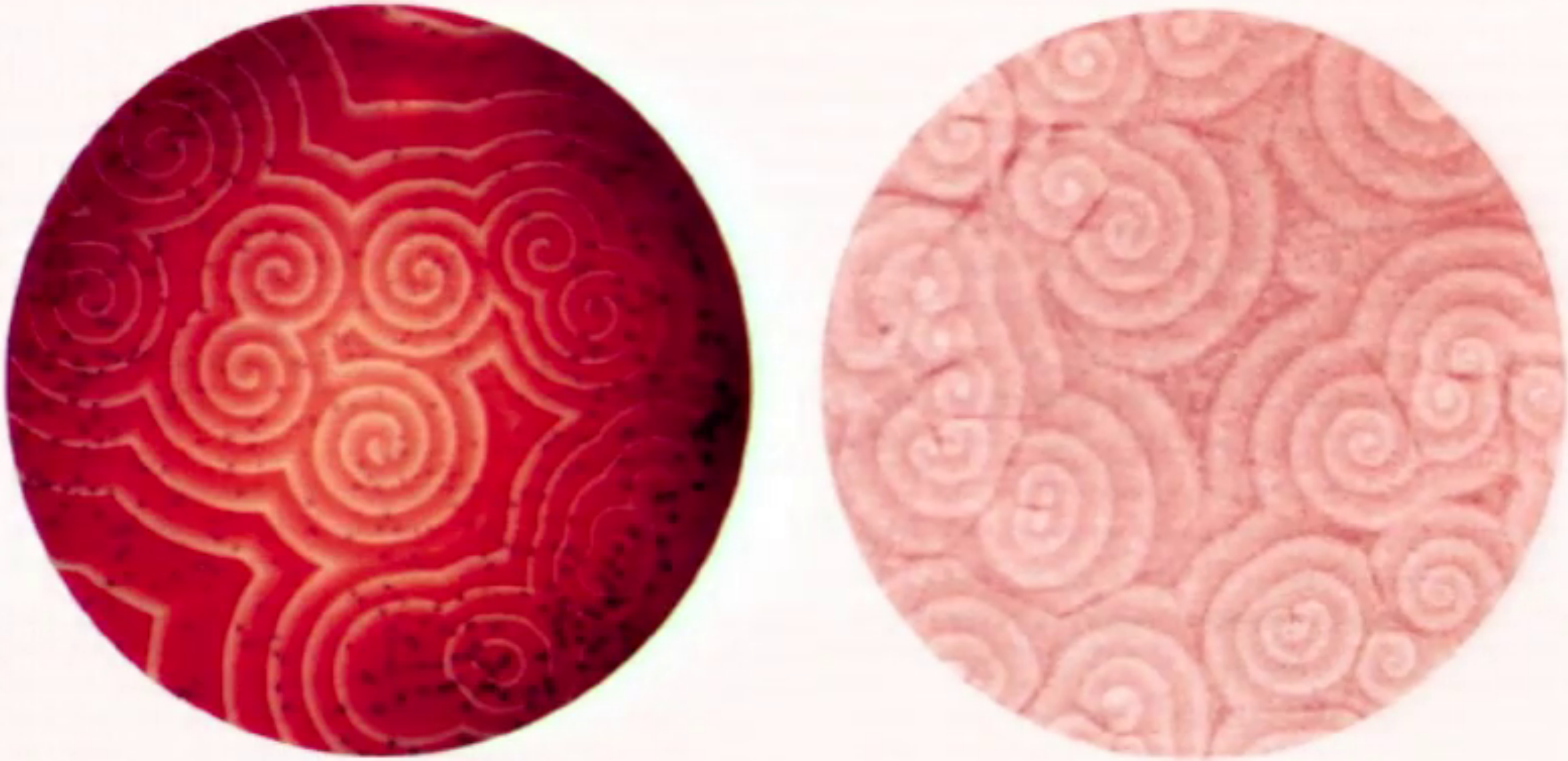




Belousov-Zhabotinsky reaction

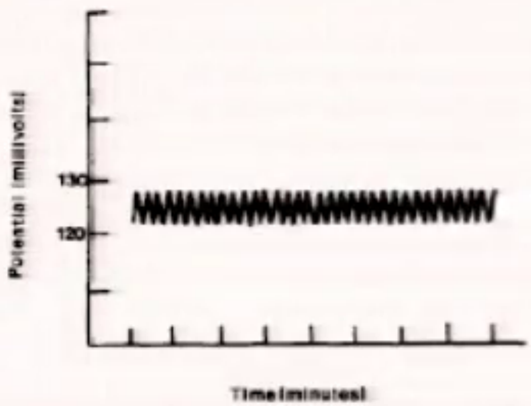


The Belousov-Zhabotinsky (BZ) reaction is an oscillating chemical reaction in which transition-metal ions catalyze oxidation of organic reductants by bromic acid.

Figure from Irving Epstein

Mixed Mode Oscillations in BZ Reaction

Hudson, Hart, Marinko (1979) J. Chem. Phys. 71:1601-1606
Homogeneous stirred tank reactor: different flow rates



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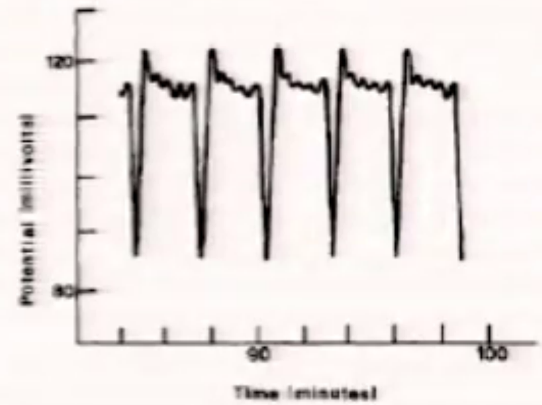

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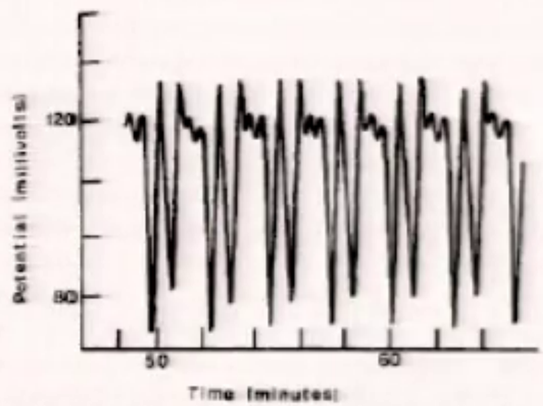

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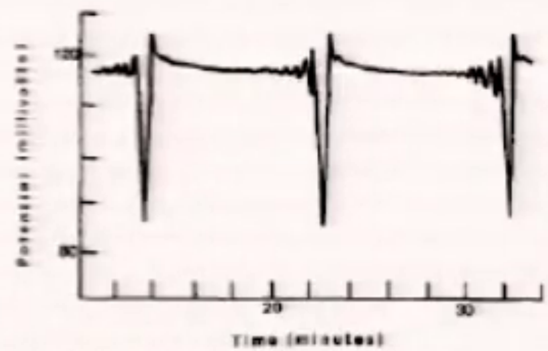


FIG. 10. Recording from bromide ion electrode; T = 25 °C; flow rate = 5.37 ml/min; Ce^{+3} catalyst.

Mixed Mode Oscillations

GSPT mechanisms that produce small amplitude oscillations

- Folded nodes
- Singular Hopf bifurcations
- Dynamic Hopf bifurcation

The Koper model is the best studied example

$$\begin{cases} \varepsilon_1 \dot{x} &= k\,y - x^3 + 3\,x - \lambda, \\ \dot{y} &= x - 2\,y + z, \\ \dot{z} &= \varepsilon_2\,(y - z), \end{cases}$$

Desroches, Guckenheimer, Krauskopf, Kuehn, Osinga and Wechselberger: SIAM Review, June, 2012

Folded Nodes

Twisting attracting and repelling slow manifolds of Koper model

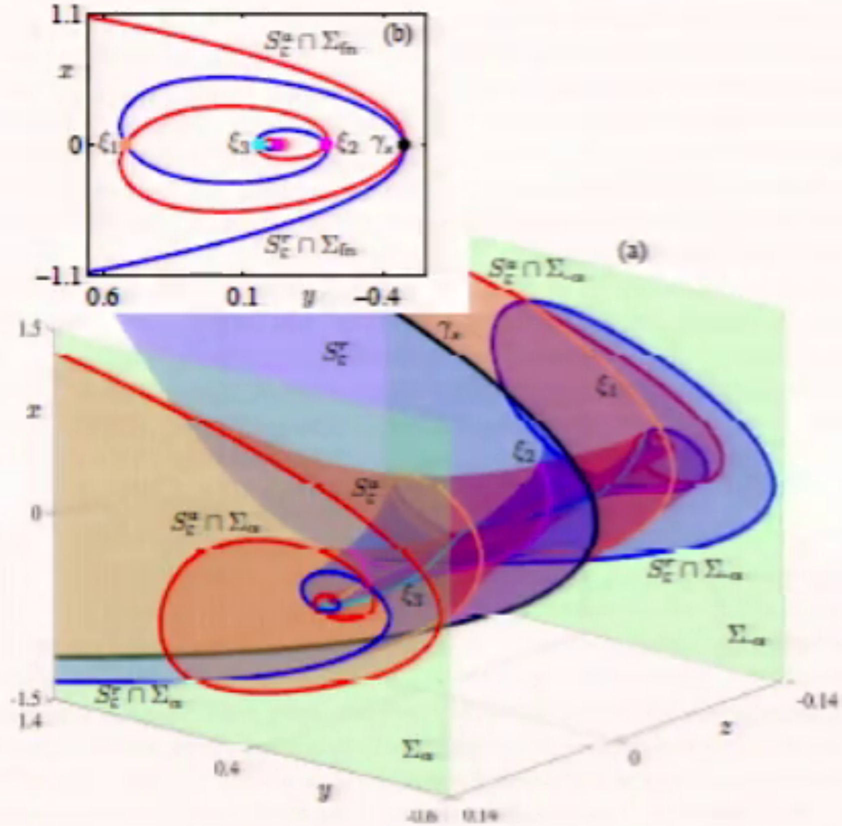
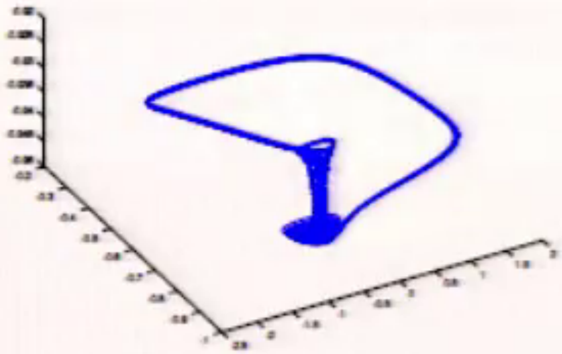
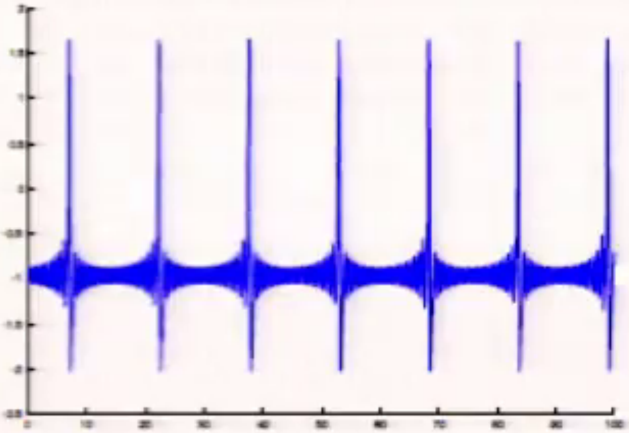


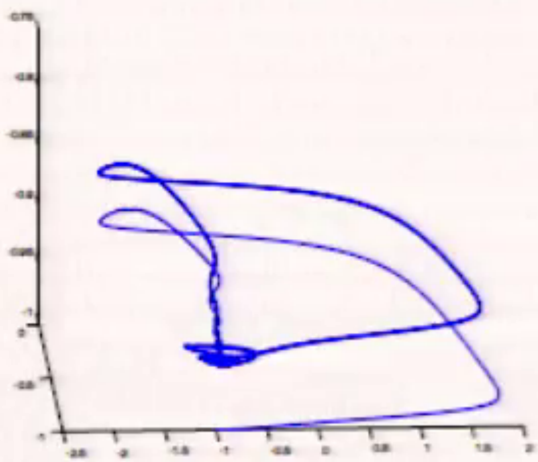
Figure: Mathieu Desroches

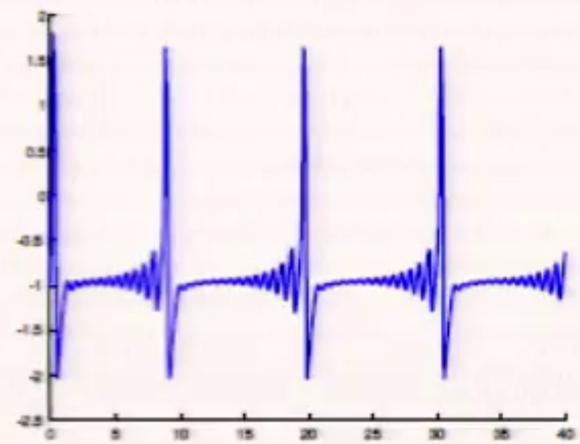
MMOs in Koper Model





Folded node: $(\lambda, k, \varepsilon_1, \varepsilon_2) = (7.5, -10, 0.1, 0.1)$

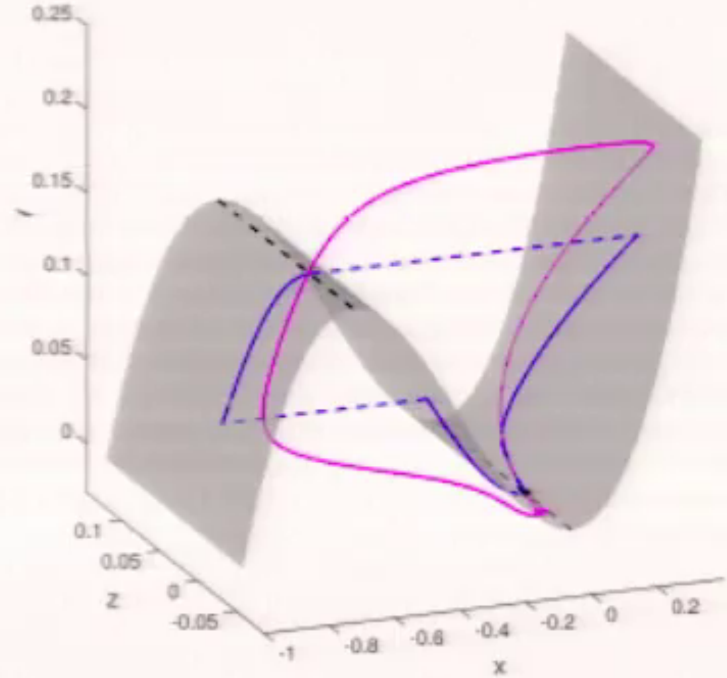




Singular Hopf: $(\lambda, k, \varepsilon_1, \varepsilon_2) = (7.5, -10, 0.1, 1)$

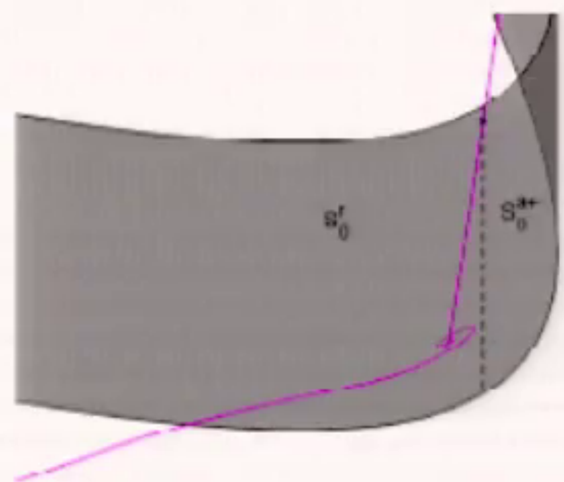
Silnikov Homoclinic orbit in Koper Model

The controversy about the deterministic or stochastic character of chemical chaos has been essentially perpetuated by numerical simulations. In fact, none among all the chemical models proposed has been able to reproduce the scenarios to chaos observed in bench experiments. – Arneodo, Argoul, Richetti: Springer Encyclopedia of Mathematics



Guckenheimer and Lizarraga

- Found elusive homoclinic orbit
- Slow-fast analysis
- Equilibrium stable/unstable manifolds follow slow manifolds
- Homoclinic orbit passes through twist region
- Transversal matching at segment boundaries



Györgyi-Field BZ Model C

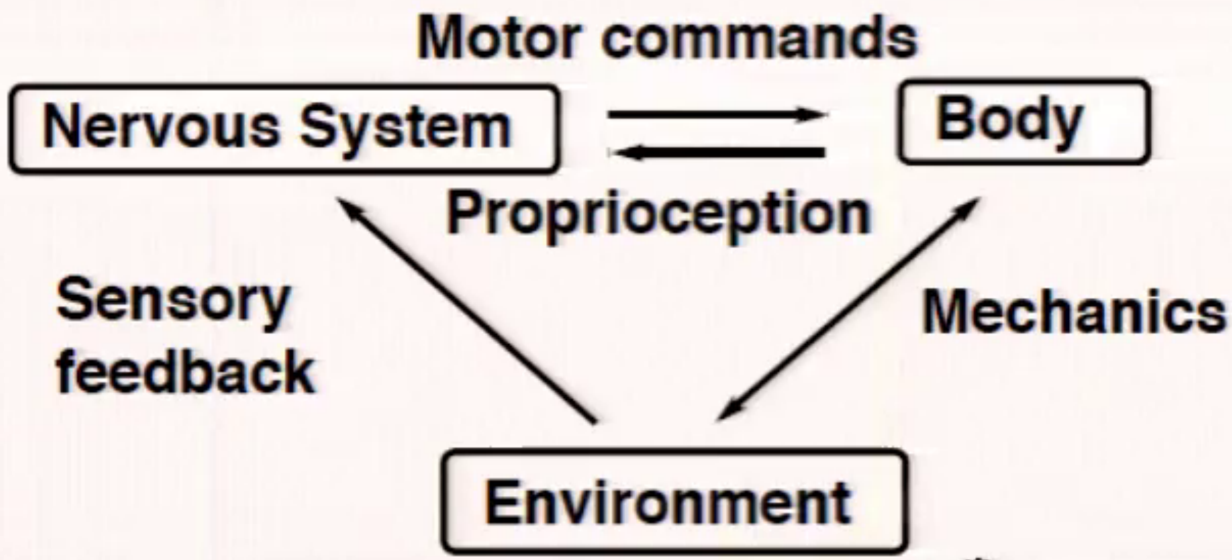
Mass action mechanism for BZ reactor

$Br^- + HBrO_2 + \{H^+\} \rightarrow 2BrMA$	$k_1 = 2.0 \cdot 10^6/(M^2 s)$
$Br^- + \{BrO_3^-\} + 2\{H^+\} \rightarrow BrMA + HBrO_2$	$k_2 = 2.0/(M^3 s)$
$2HBrO_2 \rightarrow \{BrO_3^-\} + BrMA + \{H^+\}$	$k_3 = 3.0 \cdot 10^3/(Ms)$
$\{BrO_3^-\} + HBrO_2 + \{H^+\} \rightarrow 2BrO_2^{\cdot} + \{H_2O\}$	$k_4 = 33.0/(M^2 s)$
$2BrO_2^{\cdot} + \{H_2O\} \rightarrow \{BrO_3^-\} + HBrO_2 + \{H^+\}$	$k_5 = 4.2 \cdot 10^7/(Ms)$
$Ce(III) + BrO_2^{\cdot} + \{H^+\} \rightarrow HBrO_2 + Ce(IV)$	$k_6 = 6.2 \cdot 10^4/(M^2 s)$
$HBrO_2 + Ce(IV) \rightarrow Ce(III) + BrO_2^{\cdot} + \{H^+\}$	$k_7 = 7.0 \cdot 10^3/(Ms)$
$\{MA\} + Ce(IV) \rightarrow Ce(III) + MA^{\cdot} + \{H^+\}$	$k_8 = 0.3/(Ms)$
$BrMA + Ce(IV) \rightarrow Ce(III) + Br^- + \{products\}$	$k_9 = 30.0/(Ms)$
$BrMA + MA^{\cdot} \rightarrow \{MA\} + Br^- + \{products\}$	$k_{10} = 2.4 \cdot 10^4/(Ms)$
$2MA^{\cdot} \rightarrow \{MA\} + Br^- + \{products\}$	$k_{11} = 3.0 \cdot 10^9/(Ms)$

Reproduces observed sequence of reactor states with varying flow rate

Locomotion: Data Driven Models

What do we do when models are incomplete?



Overarching problem: control

- stability
- maneuvers

Fit reduced models to observation (e.g. motion capture)

Locomotion: Data Driven Models

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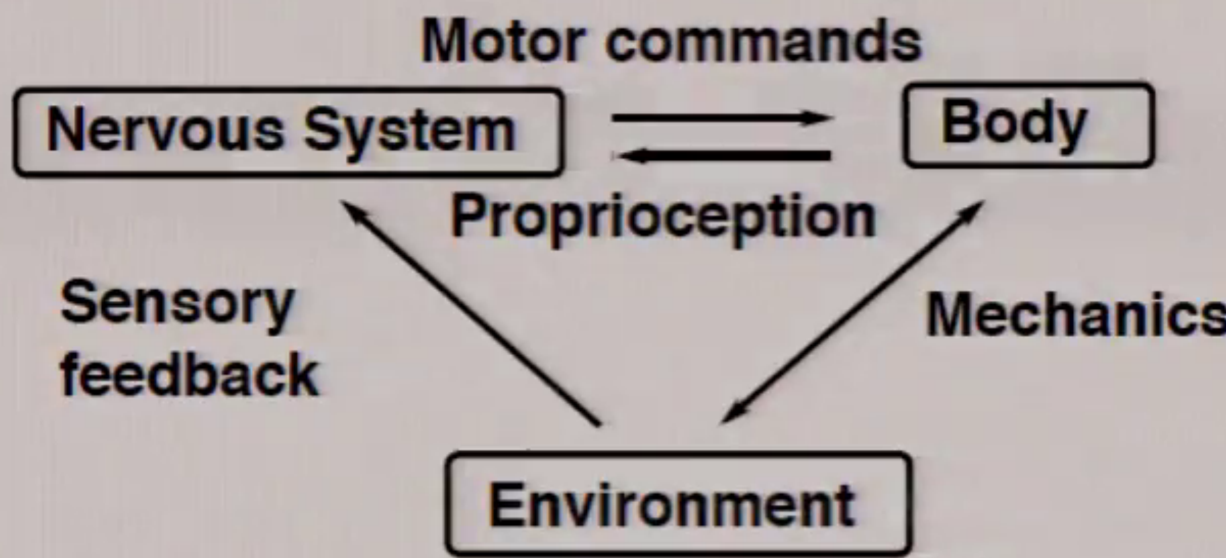

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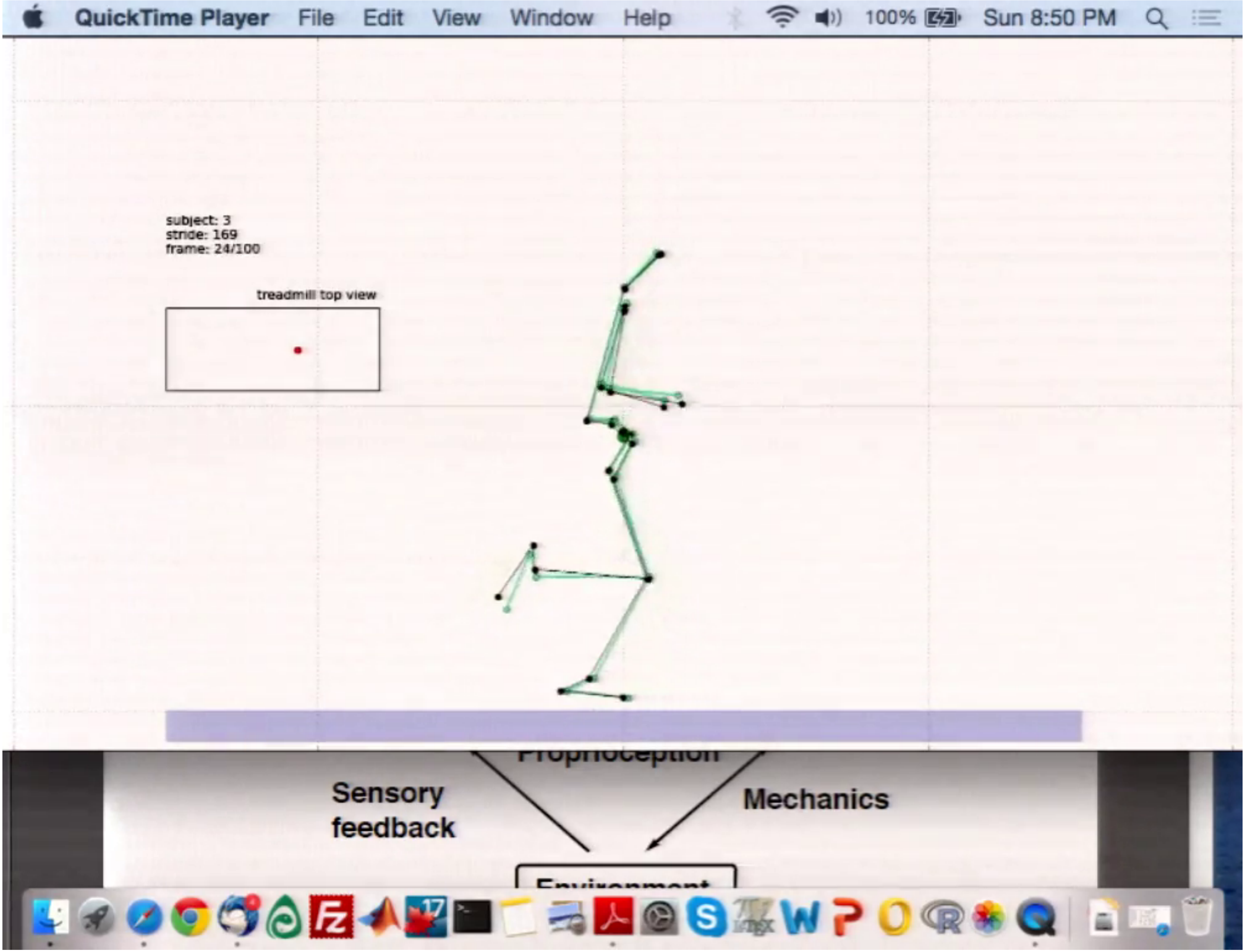
QuickTime Player
File
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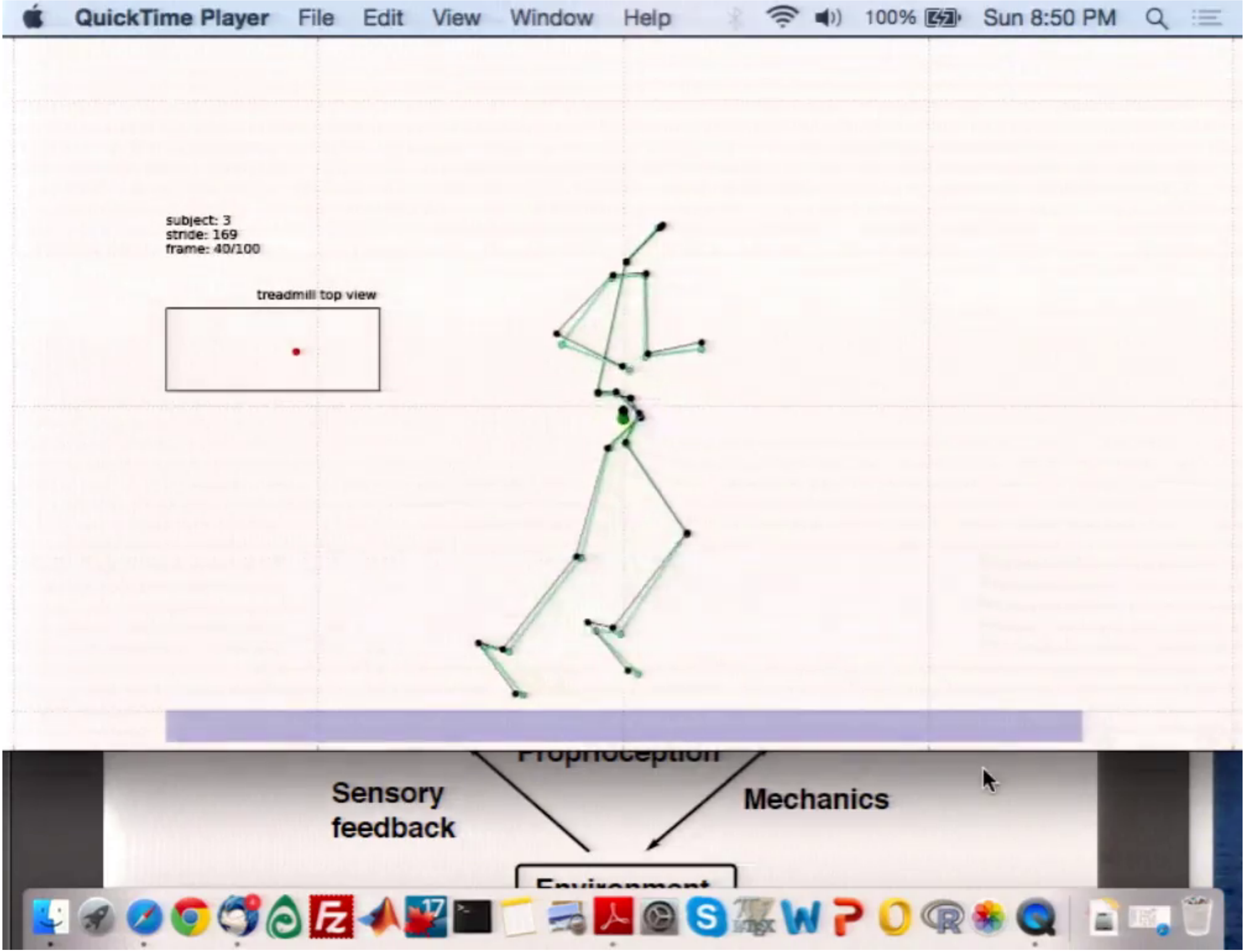
subject: 3
stride: 169
frame: 24/100
treadmill top view
Sensory feedback
Mechanics


QuickTime Player
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Sun 8:50 PM
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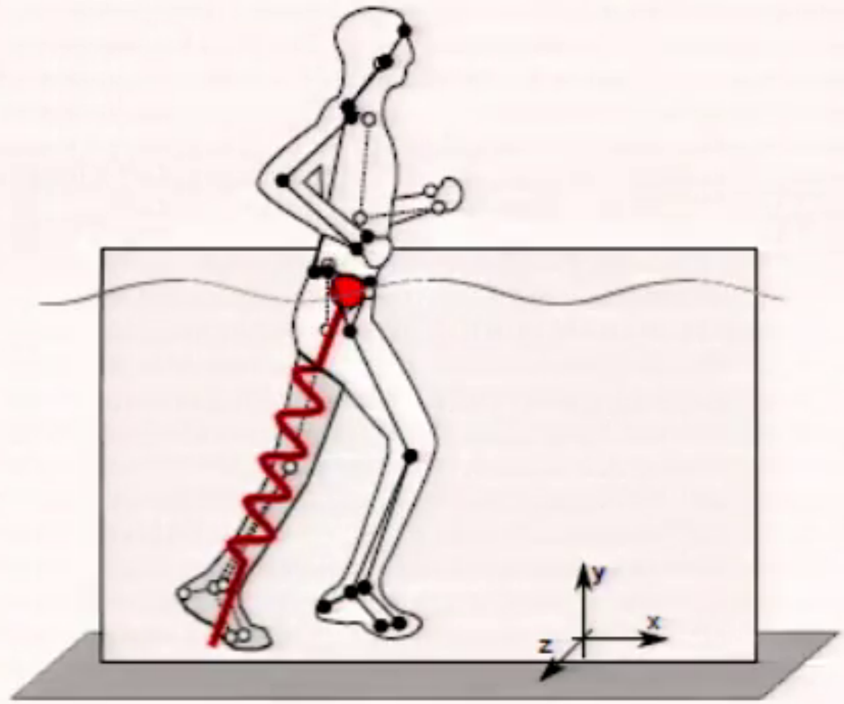
Human Treadmill Running

Data

- Motion capture: 31 markers
- Force plate in treadmill

Questions

- How do we remain upright?
- Is running predictable? For how long?
- Simple, reduced model?



Maus, Revzen, Guckenheimer, Ludwig, Reger and Seyfarth
Constructing predictive models of human running.
J. R. Soc. Interface (2015) 12:20140899.

Models and Models and Models

Templates and Anchors (Full and Koditschek, JEB 1999)

- Template: low dimensional dynamical system
- Anchor: detailed model of biomechanics and neural control

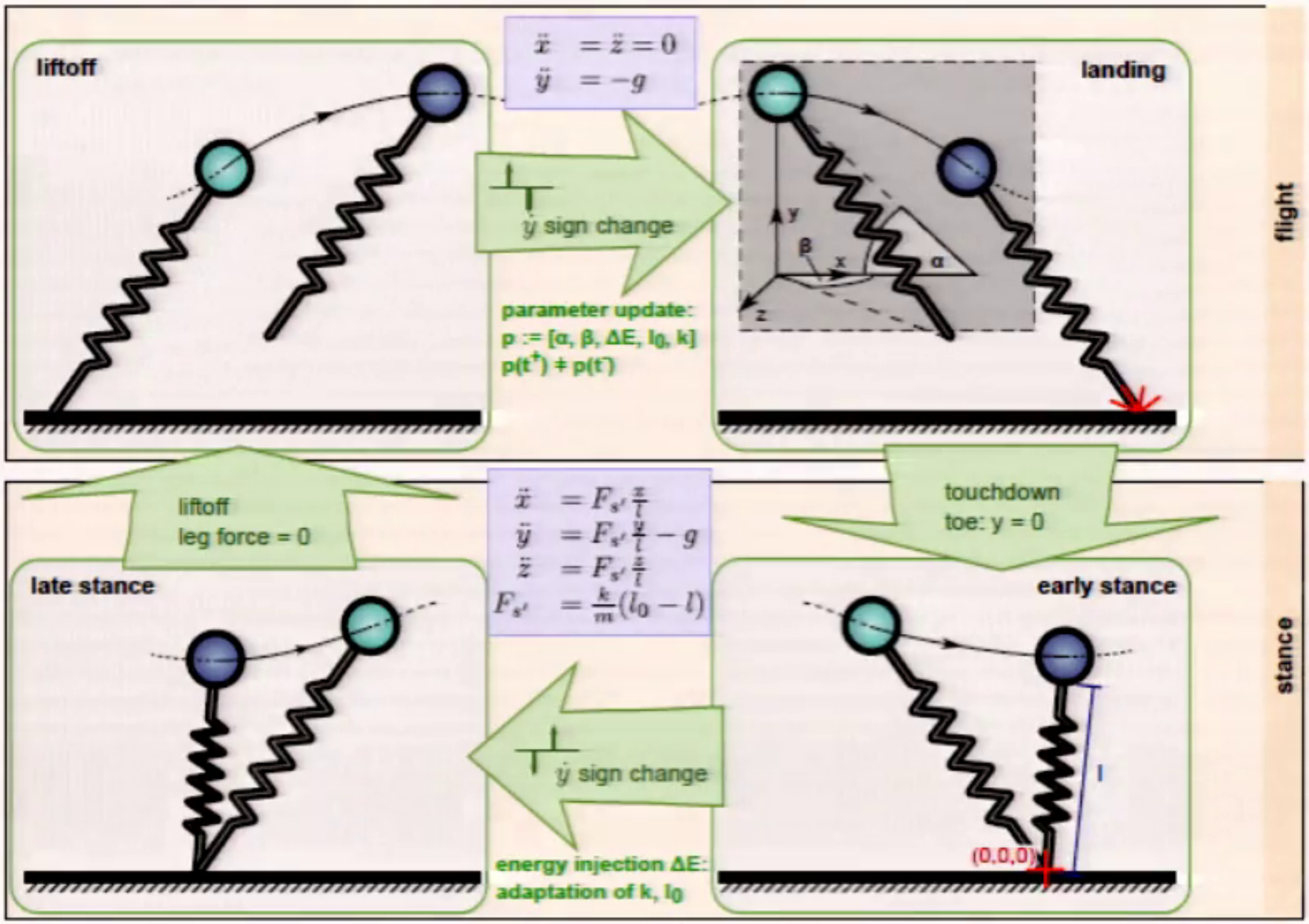
Hypotheses:

- Templates describe locomotion.
- Control is “computed” on that template.

Two templates:

- SLIP: spring loaded inverted pendulum
- Stochastic perturbation of (hybrid) stable limit cycle

Spring-mass Models (SLIP)



Is this a good mechanical template for running?

Phase Space Template

Stochastic Floquet model around periodic orbit

$$d\theta = cdt + f(\theta, u)dW$$
$$du = Audt + g(\theta, u)dW$$

with state dependent variance of Brownian motion

- SDE near periodic orbit in Floquet coordinates
- Fit stochastic return map from sample trajectories to

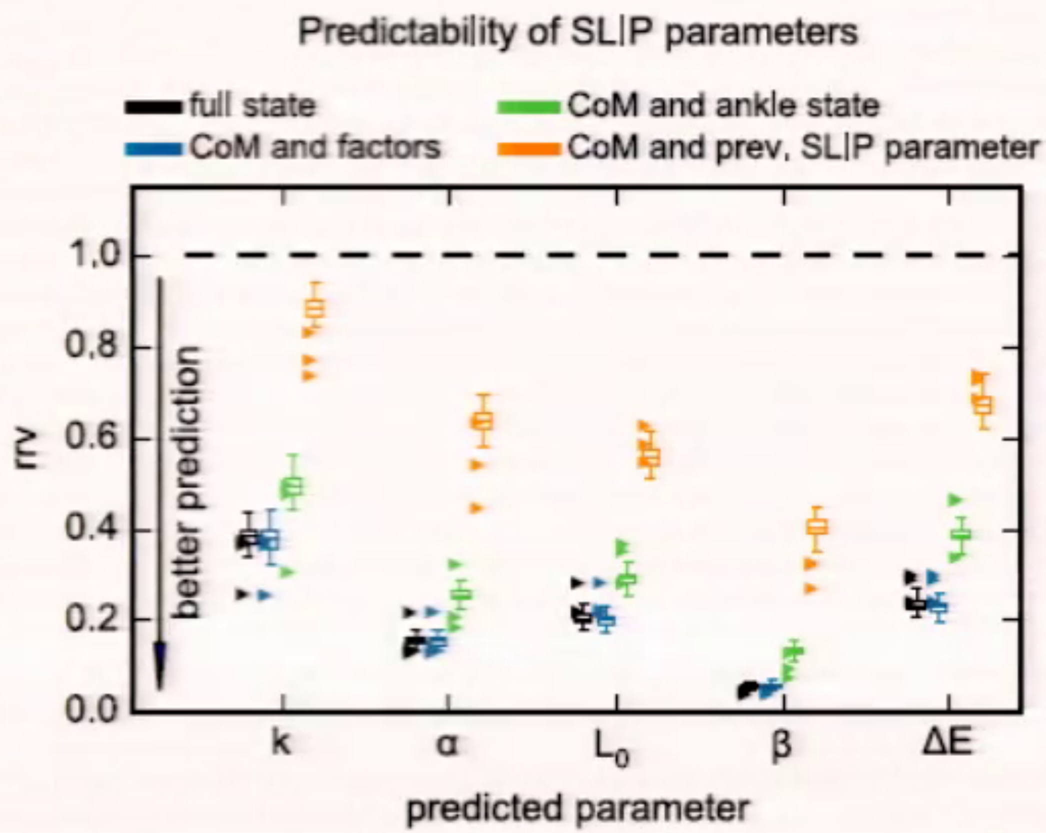
$$\sigma(u - u_0) = B(u - u_0) + N$$

- Eigenvalues of B measure (in)stability

SLIP predictability

Fit models to COM data

- Relative remaining variance of COM
- Full state model: linear controller of SLIP parameters via regression
- Factors model: reduced model via PCA
- Ankle state model: subset of observations



SLIP stability

Eigenvalues of return map

- Floquet model from data
- SLIP is unstable
- Ankle SLIP good fit