Transient spatiotemporal chaos is extensive in three reaction-diffusion networks

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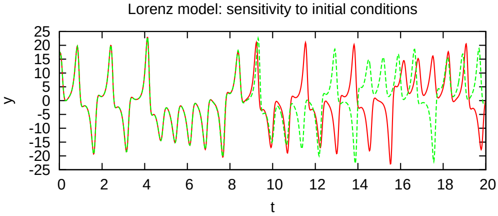
Chaos

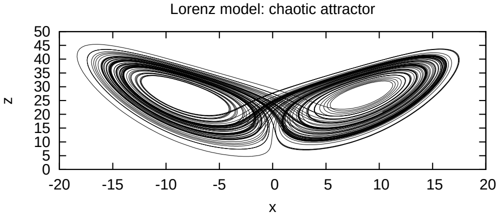
Chaotic systems are typified by:

- Sensitivity to initial conditions
- Attractor with fractional dimension

Example: Lorenz model

- $dx/dt = \sigma(y - z)$
- $dy/dt = x(\rho - z) - y$
- $dz/dt = xy - \beta z$
- $\sigma = 10, \beta = 8/3, \rho = 28$





Spatiotemporal Chaos

Some systems show disorder in both time and space

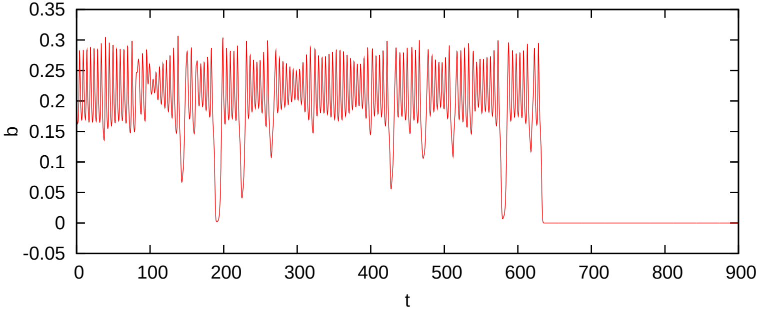
- Sensitivity to initial conditions
- No long-range spatial correlations

Examples:

- Turbulence
- Some chemical reactions
- Fibrillation in heart

Transient Chaos

- In some systems, chaos suddenly collapses after a lengthy chaotic interval
- In this case there is a chaotic saddle instead of a chaotic attractor



Reaction-diffusion networks (RDN)

- RDN are systems having a local reaction term and a diffusion term
- The domain can be continuous or a discrete network of nodes
- Example: chemical reactions
- Example: animal populations

Reaction-diffusion networks (RDN)

The general form of RDN dynamics is

$$\frac{d}{dt}\vec{y}(x) = \vec{F}(\vec{y}(x)) + D\frac{d^2}{dx^2}H\vec{y}(x).$$

Or, in discrete form

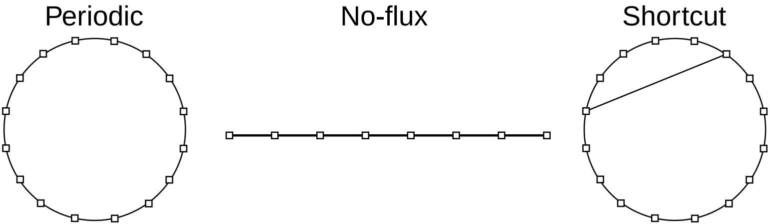
$$\frac{d}{dt}\vec{y}_i = \vec{F}(\vec{y}_i) + D\sum_{j=1}^{N} G_{ij}H\vec{y}_j$$

where typically $\sum_{j=1}^{N} G_{ij}$ is the discrete Laplacian

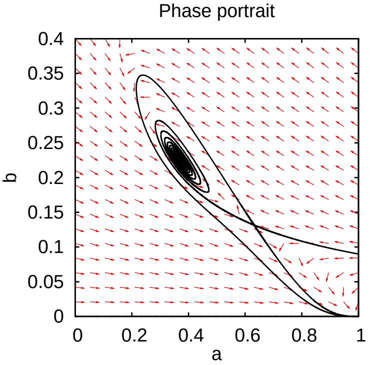
$$G_{ij} = \nabla^2_{ij} = \delta_{i,j-1} - 2\delta_{ij} + \delta_{i,j+1}.$$

Effective system size is determined by $N/\sqrt{D}$.

Boundary conditions



Gray-Scott model [GS84]



$$F_a = 1 - a - \mu a b^2$$

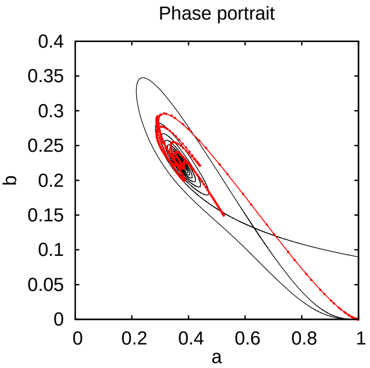
$$F_b = \mu a b^2 - \phi b$$

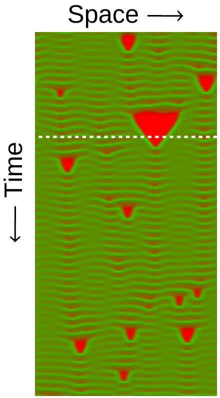
$$H = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\mu = 33.7, \phi = 2.8$$

- Represents an open autocatalytic reaction $A + 2B \rightarrow 3B$ and $B \rightarrow C$

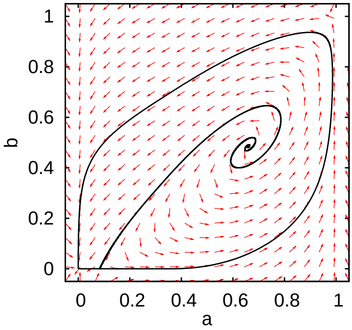
Gray-Scott model [GS84]





Bär-Eiswirth model [BE93]

Phase portrait



$$F_a = \frac{a}{\epsilon}(1-a)(a - \frac{b+\beta}{\alpha})$$

$$F_b = f(a) - b$$

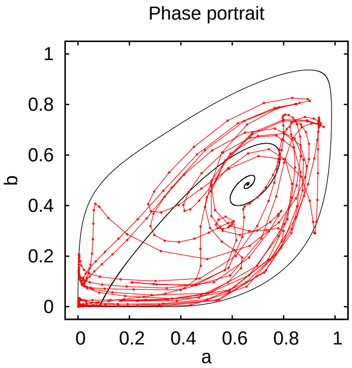
$$f(a) = \begin{cases} 0 & \text{if} \quad a < 1/3 \\ 1 - 6.75a(a-1)^2 & \text{if} \quad 1/3 \le a \le 1 \\ 1 & \text{if} \quad a > 1 \end{cases}$$

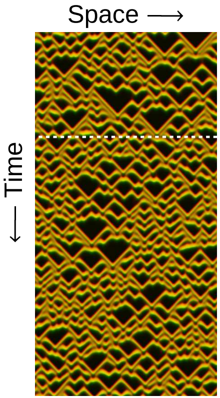
$$H = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

$$\alpha = 0.84, \beta = 0.07, \epsilon = 0.12$$

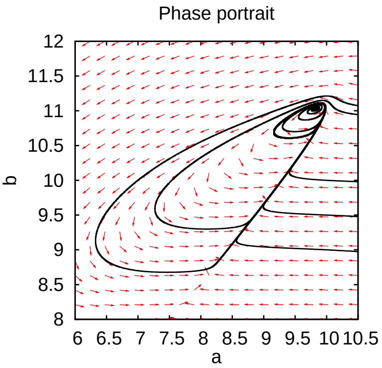
- Describes a surface reaction model for the oxidation of CO on Pt

Bär-Eiswirth model [BE93]





Wacker-Schöll model [WBS95]



$$F_a = \frac{b - a}{(b-a)^2 + 1} - \tau a$$

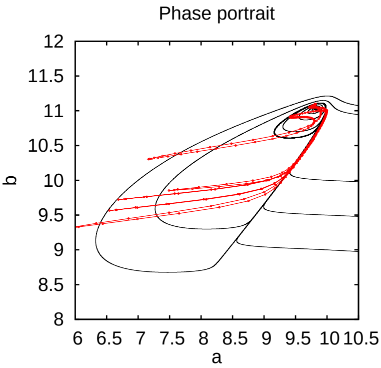
$$F_b = \alpha(j_0 - (b - a))$$

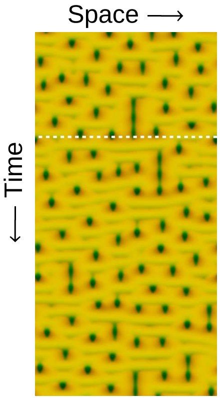
$$H = \begin{bmatrix} 1 & 0 \\ 0 & 8 \end{bmatrix}$$

$$\alpha = 0.02, \tau = 0.05, j_0 = 1.21$$

- Describes charge transport in a simplified model of layered semiconductors

Wacker-Schöll model [WBS95]





Extensivity

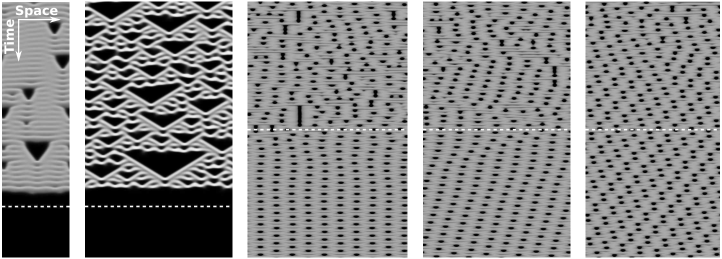
Extended chaotic systems that have no long-range interactions are expected to be uncorrelated at large length scales and therefore should behave as a sum of their parts [Rue82].

Therefore, it can be expected that:

- $D_{\mathcal{L}} \propto N/\sqrt{D}$
- $\ln \langle T \rangle \propto N/\sqrt{D}$

(these measures will be defined later on)

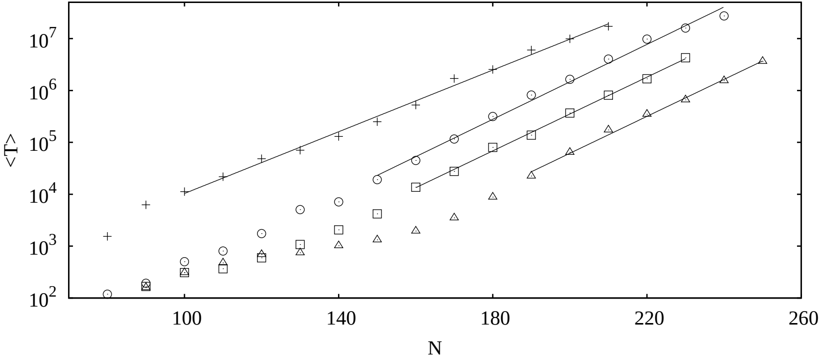
Transient Chaos



(a) (b) (c) (d) (e)

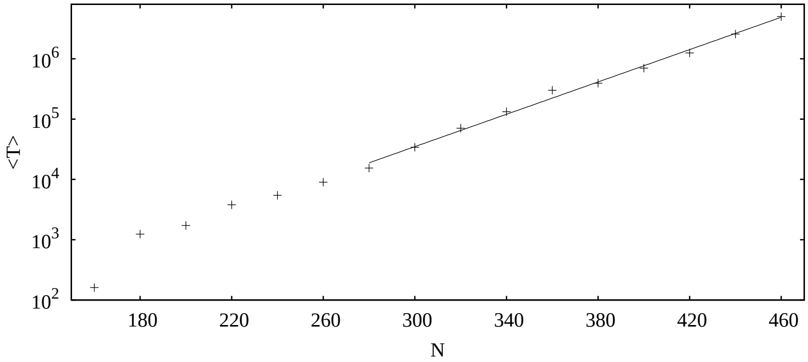
- (a) Gray-Scott, N=210
- (b) Bär-Eiswirth, N=460
- (c)-(e) Wacker-Schöll, N=500,460,420

Average Lifetime: Gray-Scott model



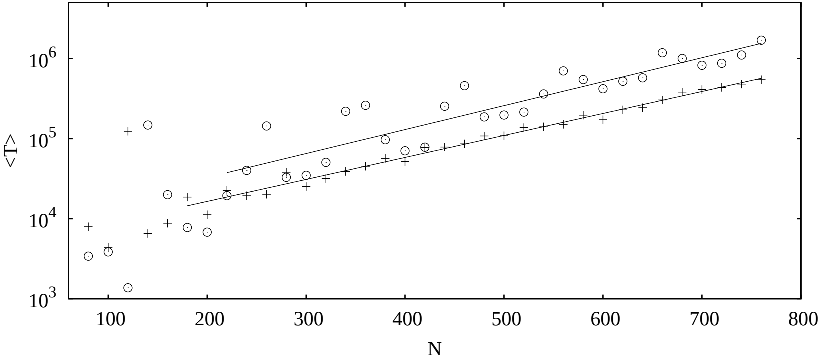
(+) no-flux (□) periodic with shortcut of length 50
(○) periodic (△) periodic with shortcut of length $N/2$

Average Lifetime: Bär-Eiswirth model



(+) no-flux

Average Lifetime: Wacker-Schöll model

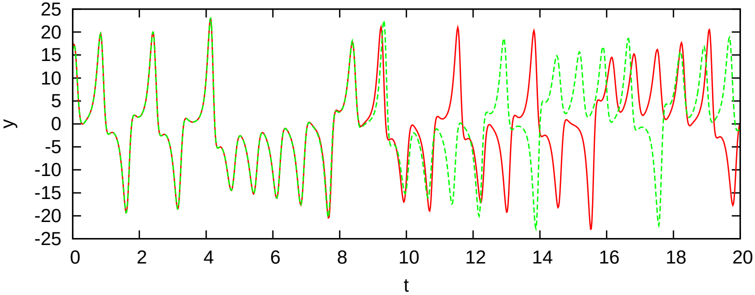


(+) no-flux
(○) periodic

Lyapunov Exponents

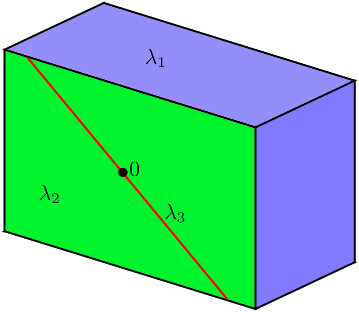
- Lyapunov exponents describe the rate at which small perturbations expand or contract
- $\epsilon\vec{v}(t) = \vec{y}'(t) - \vec{y}(t)$ where ϵ is infinitesimal
- The largest Lyapunov exponent is positive in chaotic systems

Lorenz model: sensitivity to initial conditions

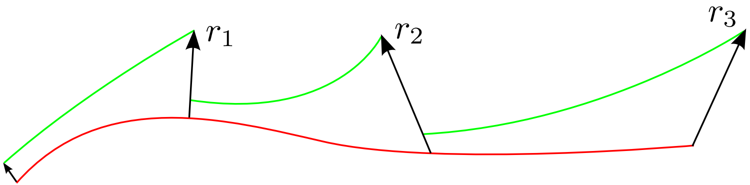


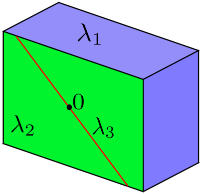
Lyapunov Spectrum

- The number of Lyapunov exponents is equal to the number of degrees of freedom.
- They describe rates of expansion of infinitesimal perturbation vectors belonging to a sequence of nested linear subspaces



First Lyapunov Exponent

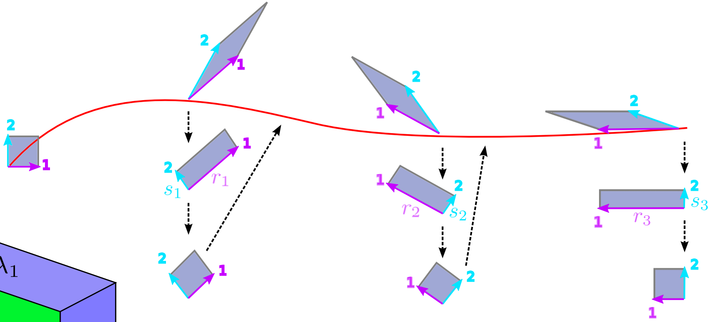


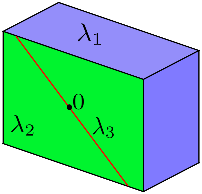


$$e^{\lambda_1 t} = \prod_i r_i$$

$$\lambda_1 = \frac{1}{t} \sum_i \log r_i$$

Second Lyapunov Exponent



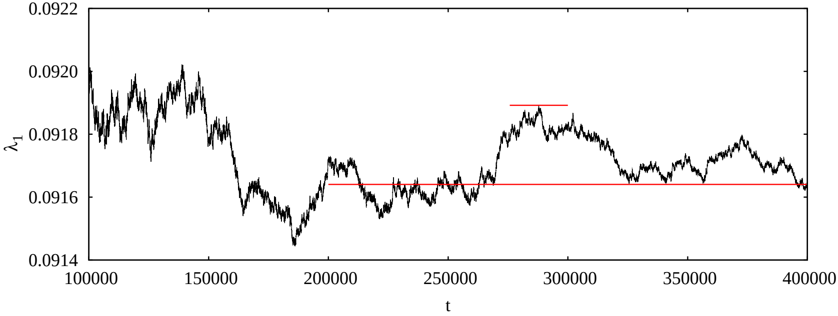


$$e^{\lambda_1 t} = \prod_i r_i \qquad e^{(\lambda_1+\lambda_2)t} = \prod_i r_i s_i$$

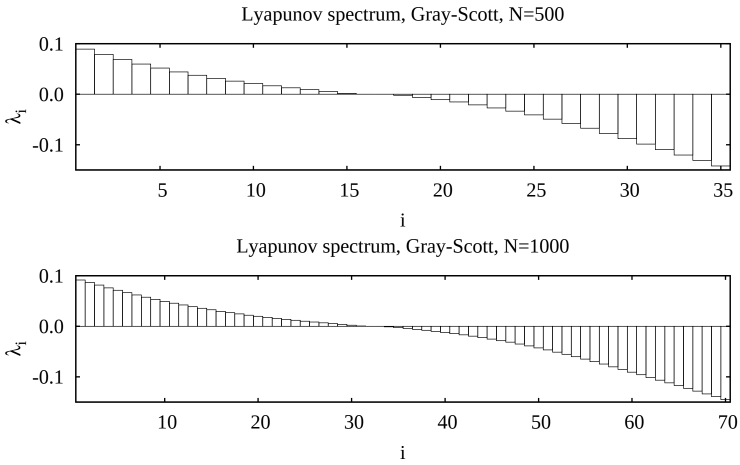
$$\lambda_1 = \frac{1}{t}\sum_i \log r_i \qquad \lambda_2 = \frac{1}{t}\sum_i \log s_i$$

Error Estimation

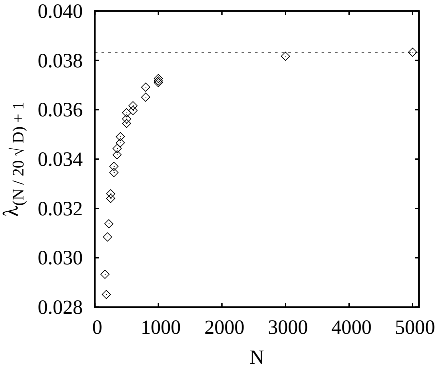
Convergence of Lyapunov exponent calculation is slow. Error is estimated to be the difference between the final value and the maximum deviation from this value during the last half of the simulation.

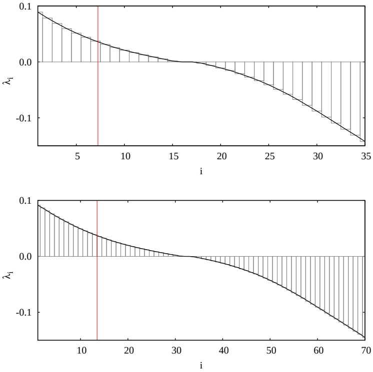


Lyapunov Spectrum



Extensivity of Lyapunov Spectrum



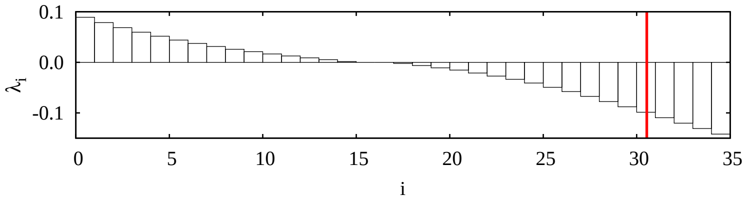


Lyapunov Dimension

The *Lyapunov dimension*, also called the *Kaplan-Yorke dimension*,

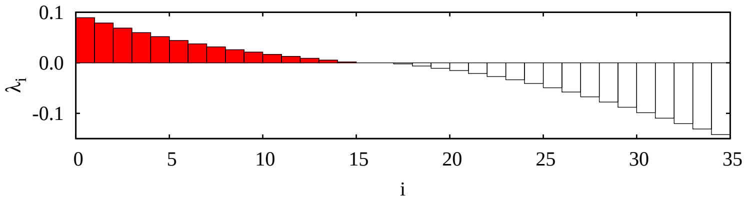
$$D_{\mathcal{L}} = j + \frac{\lambda_1 + \ldots + \lambda_j}{|\lambda_{j+1}|},$$

is conjectured to be equal to the information dimension for typical attractors [Ott02].

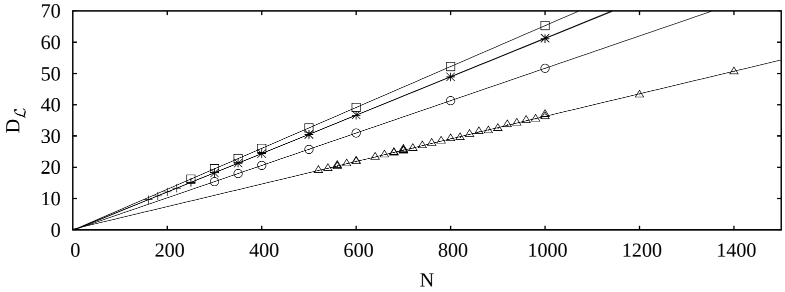


Sum of Positive Exponents

The sum of positive Lyapunov exponents, $\sum^{+}$, represents an upper bound for the Kolmogorov-Sinai entropy [Ott02].

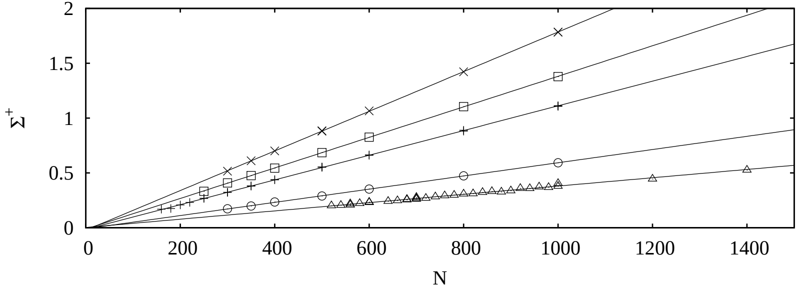


Extensivity of Lyapunov Dimension $D_{\mathcal{L}}$



(□)	Gray-Scott, $\mu = 33.5$	(×)	Bär-Eiswirth
(+)	Gray-Scott, $\mu = 33.7$	(△)	Wacker-Schöll
(○)	Gray-Scott, $\mu = 33.9$		

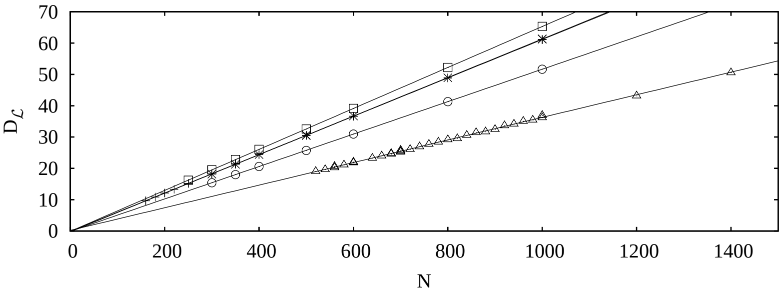
Extensivity of Sum of Positive Lyap. Exponents $\sum^+$



(□)	Gray-Scott, $\mu = 33.5$	(×)	Bär-Eiswirth
(+)	Gray-Scott, $\mu = 33.7$	(△)	Wacker-Schöll
(○)	Gray-Scott, $\mu = 33.9$		

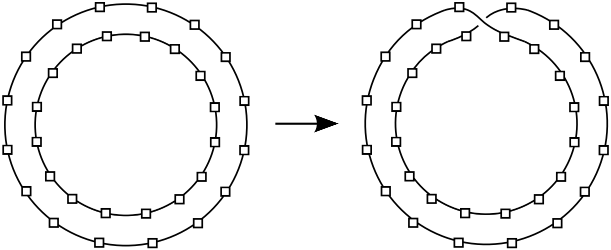
Y-Intercept of $D_{\mathcal{L}}$ vs. N

- The y-intercept of $D_{\mathcal{L}}$ vs. N should be zero for systems with periodic boundary conditions
- Why?



Y-Intercept of $D_{\mathcal{L}}$ vs. N

- Take the linear ansatz $D_{\mathcal{L}}(N) \rightarrow aN + b$ as $N \rightarrow \infty$
- For large N, $2D_{\mathcal{L}}(N) = D_{\mathcal{L}}(2N)$
- Therefore $b = 0$



- The results mostly verify this hypothesis

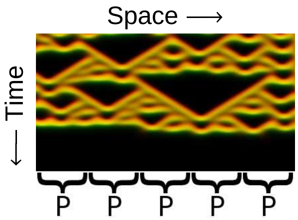
Intensive Quantities

An extensive quantity divided by size gives an intensive quantity.

- Lyapunov dimension density: [Gre99]
  $\delta_D \equiv \lim_{N\to\infty} N^{-1} D_{\mathcal{L}}$
- Log-lifetime density:
  $\delta_T \equiv \lim_{N\to\infty} N^{-1} \ln \langle T \rangle$

Intensive Quantities

So, what do these quantities mean? Consider transient chaos.



Probability of collapse is $P^{N/\xi}$, so lifetime takes the form [TL08]

$$\langle T \rangle \sim P^{-N/\xi} = e^{-(\ln P)\frac{N}{\xi}},$$

and log-lifetime density takes the form

$$\delta_T = \frac{-\ln P}{\xi}.$$

Intensive Quantities

$$\delta_T = \frac{-\ln P}{\xi}$$

- The quantity δ_T apparently has units of number of coins tossed per unit length
- δ_T is computable whereas P and ξ are only defined intuitively

A New Quantity

δ_T has dimensions of coins tossed per unit length and δ_D has units of active degrees of freedom (i.e. attractor dimension) per unit length. Taking their ratio eliminates the length units:

$$\sigma \equiv \delta_T/\delta_D.$$

This quantity has units of coins tossed per active degree of freedom.

A New Quantity

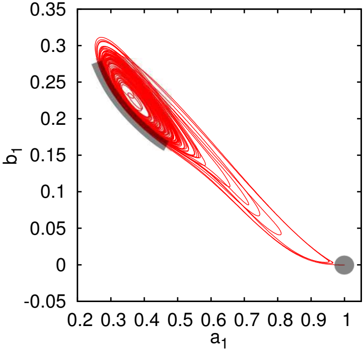
And what does σ mean? For large N,

$$\begin{aligned} \delta_T &= N^{-1} \ln \langle T \rangle \\ \langle T \rangle^{-1} &= e^{-N\delta_T} \\ &= e^{-N\delta_D \sigma} \\ &= e^{-D_{\mathcal{L}} \sigma} \\ &= (e^{-\sigma})^{D_{\mathcal{L}}}. \end{aligned}$$

This leads to an intuitive argument for understanding the escape rate from the chaotic saddle.

Escape Route

Each time the chaotic trajectory ”orbits” around the chaotic saddle, it has an opportunity of escaping into a non-chaotic state. Think of a ”hole” in the chaotic saddle.



Escape Route

$$\langle T \rangle^{-1} = (e^{-\sigma})^{D_{\mathcal{L}}}$$

- Ignoring the fact that the chaotic saddle has fractal dimension;
- Ignoring the fact that $D_{\mathcal{L}}$ is only approximately equal to the saddle dimension;
- Considering the saddle as being approximately a set product of smaller saddles;
- Then $(e^{-\sigma})^{D_{\mathcal{L}}}$ is the volume of a hypercube of width $e^{-\sigma}$ and dimension $D_{\mathcal{L}}$.
- So, can we find a feature in the chaotic saddle that is size $e^{-\sigma}$?

Escape Route

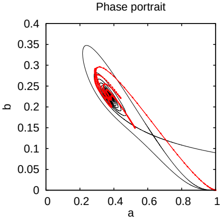
Well, it's not quite that easy.

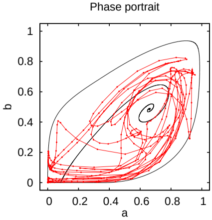
$$\langle T \rangle^{-1} = (e^{-\sigma})^{D_{\mathcal{L}}}$$

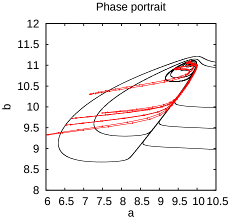
- $e^{-\sigma}$ is actually the **geometric mean** of the hole's widths along each dimension
- The trajectory passes by certain areas more often than others, and this needs to be taken into account
- So, the interpretation is not so clear cut

Escape Route

Gray-Scott	Bär-Eiswirth	Wacker-Schöll
$e^{-\sigma} \approx 0.28$	$e^{-\sigma} \approx 0.62$	$e^{-\sigma} \approx 0.85$

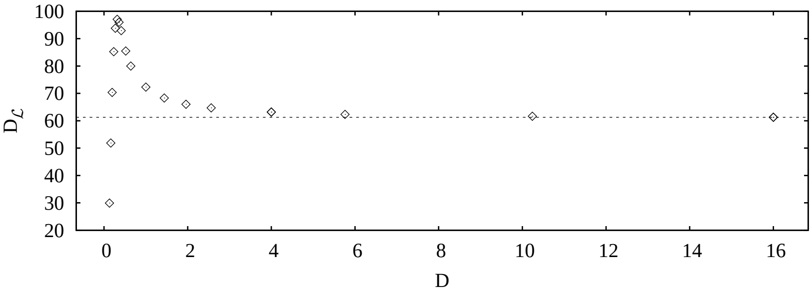






Discretization Error

- Effective system size is determined by $N/\sqrt{D}$
- Small N $\implies$ more efficient computation
- Small D $\implies$ more discretization error
- What is the limit?



Conclusions

- $\ln \langle T \rangle$, $D_{\mathcal{L}}$, and $\sum^{+}$ grow linearly with size
- $D_{\mathcal{L}}$ and $\sum^{+}$ are constant for $N/\sqrt{D}$ fixed
- Boundary conditions affect x-intercept (but not slope) of $\ln \langle T \rangle$ and $D_{\mathcal{L}}$ vs. N
- Y-intercept for $D_{\mathcal{L}}$ vs. N should be zero for periodic boundary conditions
- The quantity $e^{-\sigma}$ may relate to escape routes from the chaotic saddle

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