## Experimental Mathematics in dynamical Systems

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DDAYS'14, Badajoz
12-14 November, 2014

## Outline

- Our point of view and a fast review of our current research
(1) Numerical techniques to explore complex behaviors
(2) Experimental mathematics: high-precision and more ...
(3) Need to mixing techniques (so collaborations): "bailar juntos"
(4) Need to prove some results: CAP
(5) Need to use "problem"-specific techniques: kneading plots


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## Numerical tools (the need of a lot of techniques ...)

- General chaos indicators:

MLE, Lyapunov exponents, MFGN , FL OFLI2, FMA ...

- Computation of invariap
- Continuation of er dic its ..: MATCOMT, AL O, CONTID OMb. A De cand R drí eez 2012 3) ...
- Bifur th - s : Mratcon AU $0, \ldots$
- Prti re nana- d dynamic ine sato

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Dutv-c le di yran (B. and Chilh oov 01
Spe ifi ohen nena: Sh ups ind polagival changes (B., Blesa,

- Detá ed scudies
- Arbi ar prec io

UM IIC L-M ROSCOPE (Abad, B. and Dena, 2012)

- go s stures CAP: Rigorous DATA BASE of periodic orbits (C IPD) (B., Dena, Tucker, 2014), Hyperchaos (2014), ...


## What is TIDES?

: a Taylor series Integrator for Differential EquationS

- Taylor series method using Variable-Stepsize Variable-Order formulation and extended formulas for the variational equations.
- Free numerical software based on extended Taylor series method: TIDES*.
- Extremely easy to use via a MATHEMATICA preprocessor. NOW INCLUDED IN SAGE (2014)!!!
- Automatic construction of Fortran or C codes for solving ODEs
- Automatic construction of C codes for solving solutions of ODEs and variational equations up to any order (and sensitivities with respect to any parameter up to any order)
- Easy to use arbitrary precision (do you need 500 digits?, 1000?)

Where?: http://cody.unizar.es/software or email: tides.taylor@gmail.com, rbarrio@unizar.es

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## Experimental mathematics in Dynamical Systems

## Origin of the discipline in Spain

$\longrightarrow$ Prof. Carles Simó (Universidad de Barcelona)


## Experimental mathematics (?) ${ }^{\dagger}$

"Experimental mathematics" has emerged in the past 25 years or so to become a competitive paradigm for research in the mathematical sciences.

So what exactly is "experimental mathematics"? While several definitions have been offered, perhaps the most succinct definition is given in the Borwein-Devlin book The Computer as Crucible:

> Experimental mathematics is the use of a computer to run computations - sometimes no more than trial-and-error tests - to look for patterns, to identify particular numbers and sequences, to gather evidence in support of specific mathematical assertions that may themselves arise by computational means, including search.

Here we should distinguish "experimental mathematics" from "computational mathematics" and "numerical mathematics." While there is no clear delineation, the latter two terms generally encompass computational methods for concrete applied mathematics and engineering applications.

[^1]
## Experimental mathematics: books



David H. Bailey
and
Jonathan M. Borwein
PSiprices


## Progress of Scientific Supercomputers: Data from the Top500 List



## Experimental math: Discovering new mathematical results by computer

- Compute various mathematical entities (limits, infinite series sums, definite integrals) to high precision, typically 100-1000 digits.
- Use algorithms such as PSLQ to recognize these entities in terms of wellknown mathematical constants.
- When results are found experimentally, seek to find formal mathematical proofs of the discovered relations.
Many results have recently been found using this methodology, both in pure mathematics and in mathematical physics.

```
Decrease of log 10(min |yi|) in multipair PSLQ run
```

(:300

## Computing: <br> The Third Mode of Scientific Discovery



Theory

## Experiment



## Computing

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## References

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R．Barrio，M．Lefranc，M．A．Martinez，S．Serrano，Symbolic dynamical unfolding of spike－adding bifurcations in chaotic neuron models，Europhysics Letter（EPL）， submitted， 2014.
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R．Barrio，M．A．Martinez，S．Serrano，A．Shilnikov，Macro－and micro－chaotic structures in the Hindmarsh－Rose model of bursting neurons，Chaos：An Interdisciplinary Journal of Nonlinear Science 24 （2），023128， 2014.
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R．Barrio，A．Shilnikov，Parameter－sweeping techniques for temporal dynamics of neuronal systems：case study of Hindmarsh－Rose model，The Journal of Mathematical Neuroscience（JMN） 1 （1），1－22， 2011.

## Mathematical neuron models

The Hodgkin-Huxley model is a mathematical model that describes how action potentials in neurons are initiated and propagated.
Alan Lloyd Hodgkin and Andrew Huxley described the model in 1952 to explain the ionic mechanisms underlying the initiation and propagation of action potentials in the squid giant axon. They received the 1963 Nobel Prize in Medicine for this work.


Other mathematical models:

## The leech heart interneuron model



[^2]
## The leech heart interneuron model



- Onion-like structures.
- Spike-adding bifurcations $\longrightarrow$ UPOs foliated in the attractor $\longrightarrow$ ??


## The Hindmarsh and Rose model

## The Hindmarsh and Rose model (1984)

A phenomenological system of ODEs for modeling bursting and spiking oscillatory activities in isolated neurons:

$$
\begin{align*}
\dot{x} & =y-a x^{3}+b x^{2}-z+l \\
\dot{y} & =c-d x^{2}-y  \tag{1}\\
\dot{z} & =\varepsilon\left(s\left(x-x_{0}\right)-z\right)
\end{align*}
$$

- $x$ is treated as the membrane potential, while $y$ and $z$ describe some fast and slow gating variables for ionic currents.
- Slow "activation" of $z$ is due to the small parameter $0<\varepsilon \ll 1$.
- The parameters are typically set as $a=1, c=1, d=5, s=4$, $x_{0}=-1.6$ and $\varepsilon=0.01$.
- A key parameter is the external applied current $I$.


## Fast-slow decomposition



## Fast-slow decomposition

## Bursting classification (Rinzel-Izhikevich)

|  |  | bifurcations of limit cycles |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | saddle-node on invariant circle | saddle homoclinic orbit | supercritical AndronovHopf | fold limit cycle |
|  | saddle-node (fold) | fold/ circle | fold/ homoclinic | fold/ <br> Hopf | fold/ fold cycle |
|  | saddle-node on invariant circle | circle/ circle | circle/ homoclinic | circle/ Hopf | circle/ fold cycle |
|  | supercritical <br> Andronov- <br> Hopf | Hopf/ circle | Hopf/ homoclinic | Hopf/ Hopf | Hopf/ fold cycle |
|  | subcritical <br> Andronov- <br> Hopf | subHopf/ circle | subHopf/ homoclinic | subHopf/ Hopf | subHopf/ fold cycle |

## Square-wave bursting (fold/hom bursting)

## But ... why and where is the chaotic behavior?




## Scheme of the macroscopic chaotic structures ( $\forall \varepsilon$ )



## The Hindmarsh and Rose model: bifurcation analysis



## Codimension-two homoclinic bifurcation points

- Inclination flip

- Inclination flip + orbit flip homoclinic bifurcations



## The Hindmarsh and Rose model



## Hindmarsh and Rose: bifurcation sketch




## Topological templates

Given a three-dimensional (3D) hyperbolic chaotic flow $\Phi_{t}$, Birman and Williams define the following equivalence relation which identifies points of the invariant set $\Lambda$ having the same asymptotic future:

$$
\forall x, y \in \Lambda, \quad x \sim y \Leftrightarrow \lim _{t \rightarrow \infty}\left\|\Phi_{t}(x)-\Phi_{t}(y)\right\|=0
$$

The Birman-Williams theorem states:
(1) In the set of equivalence classes, the hyperbolic flow $\Phi_{t}$ induces a semi-flow $\bar{\Phi}_{t}$ on a branched manifold $\mathcal{K}$. The pair $\left(\bar{\Phi}_{t}, \mathcal{K}\right)$ is called a template, or knot-holder
(2) Unstable periodic orbits of $\Phi_{t}$ in $\Lambda$ are in one-to-one correspondence with unstable periodic orbits of $\left(\bar{\Phi}_{t}\right.$ in $\left.\mathcal{K}\right)$. Moreover, every link of unstable periodic orbits of $\left(\Phi_{t}, \Lambda\right)$ is isotopic to the corresponding link of $\left(\bar{\Phi}_{t}, \mathcal{K}\right)$.

## Topological templates



Left: two periodic orbits of periods 1 and 4 embedded in a strange attractor; Right: a link of two knots that is equivalent to the pair of periodic orbits up to continuous deformations without crossings.

## Topological templates: subtemplates



(b)

$$
0 \rightarrow 0
$$

Forbidden


## The Hindmarsh and Rose model: chaotic attractors



## Topological templates: Hindmarsh and Rose model



## Topological templates: Hindmarsh and Rose model



## Topological templates: Hindmarsh and Rose model

b M1 M2 M3 M4 M5


The templates follows the "onion" structure.

\& Proper grammar of the symbolic sequences
$\longrightarrow$ (forbidden symbolic sequences)

## Topological templates: successive Cantor structures

$$
0 \rightarrow 0
$$

$$
0 \rightarrow 0 \quad \text { Forbidden } \quad 1 \rightarrow 0 \rightarrow 0
$$



Theoretical framework for the "onion-bulb" chaotic structures

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## References

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## Playing with hyperchaos

Classical hyperchaos was invented by Sinai (around 1978). He showed that billiards colliding in 3D produce maximal chaos, that is, possess $n-1$ positive Lyapunov characteristic exponents.

Ya.G. Sinai, Appendix to the translation of S. Krylov, Works on the Foundations of Statistical Physics, Princeton University Press, Princeton, 1980.

For simple dissipative system with hyperchaos, that is, more than one direction of divergence of trajectories the first system was introduced by O. Rössler (1979).
O. E. Rossler, An equation for hyperchaos, Physics Letters A, 71, 155-157, 1979.

The occurrence of hyperchaotic behavior has been found in an electronic circuit (Matsumoto et al, 1986), NMR laser (Stoop et al, 1988), in a semi-conductor system (Stoop et al, 1989) and in a chemical reaction system (Eiswirth et al, 1992).
M. Eiswirth, Th.-M. Kruel, G. Ertl and F. W. Schneider, Hyperchaos in a chemical reaction, Chemical Physics Letters, 193 (4), 305, 1992.
T. Matsumoto, L. O. Chua and K. Kobayashi, Hyperchaos: laboratory experiment and numerical confirmation, 'IEEE Transactions on Circuits and Systems, CAS-33 (11), 1143-1147, 1986.
R. Stoop, J. Peinke, J. Parisi, B. Rohricht and R. P.Hubener, A p-Ge semiconductor experiment showing chaos and hyperchaos, Physica D, 35, 425-435, 1989.

## Experimental Hyperchaos

## Electronic circuits

T. Kapitaniak, L. Chua, G. Zhong, Experimental Hyperchaos in Coupled Chua's Circuits, IEEE Transactions on Circuits and

Systems, 41 (7), 1994.


Fig. 1. Five identical coupled Chua's circuits forming a ring.

 axis is $v_{C 1}^{(3)}, 1 \mathrm{~V} /$ /div, (b) $v_{C 1}^{(1)}$, versus $v_{C(3)}^{(3)}$, Horizontal axis is $v_{C 2}^{(1)}, 200 \mathrm{mV} /$ div, Verical axis is $v_{C 2}^{(3)}, 200 \mathrm{mV} / \mathrm{div}$, (c) $v_{C 1}^{(1)}$ versas $v_{C 2}^{(3)}$, Horizontal axis is $v_{C 1}^{(1)}, 1$ V/div, Vertical axis is $v_{C 2}^{(3)}, 200 \mathrm{mV} / \mathrm{div}$,

## Playing with hyperchaos

But ... in several simulations ${ }^{\S}$ ALWAYS (?) quite noisy


- So, chaotic?
- Hyperchaotic?
- WHAT?

[^3]
## Playing with hyperchaos

Biparametric study of the 4D Rössler system

$$
\left\{\begin{array}{l}
\dot{x}=-(y+z) \\
\dot{y}=x+a y+w \\
\dot{z}=b+x z \\
\dot{w}=-c z+d w
\end{array}\right.
$$

where we fix the values of parameters $b=3.0$ and $d=0.05$, and we allow the values of $a$ and $c$ change.


## Playing with hyperchaos

## Biparametric study of the 4D Rössler system (Lyapunov exponents based)



## Playing with hyperchaos

## Biparametric study of the 4D Rössler system (Lyapunov exponents based)

... and now with a long transient time + larger precision +


## STILL NOISY !!!!

## ... and now some theorems (CAP)

Extensive numerical studies yield us to find many approximate periodic orbits for $P$. For some pairs of these orbits we could find approximate heteroclinic connections on which we will built chaotic dynamics.

$$
\begin{aligned}
p_{1}^{8} & =(-104.32937253702462,0.028756669726685443,44.645081351998819), \\
p_{2}^{8} & =(-104.26664163365506,0.028773972266421831,44.640115482927115), \\
p_{3}^{8} & =(-104.42324539012806,0.028730815749171541,44.678254866134068), \\
p_{4}^{16} & =(-104.39575243552828,0.028738382959034744,44.666264617071981), \\
q_{1}^{12} & =(-103.69667754570543,0.028932144798038389,44.407870627484129), \\
q_{2}^{14} & =(-103.37098255164607,0.029023312473829044,44.284349486019579) .
\end{aligned}
$$

The points $p_{i}^{j}$ are approximate periodic points for $P$ of period $j$ with one-dimensional unstable manifold. The points $q_{i}^{j}$ are approximate periodic points of period $j$ with two-dimensional unstable manifold.

## ... and now some theorems (CAP)

This numerical study $\longrightarrow$ generates hypothesis and conjectures

Now it is time to state results :-)

- Defining the Poincaré section

$$
\Pi=\left\{(x, 0, z, w) \in \mathbb{R}^{3} ; \dot{y}=x+z<0\right\}
$$

and $P: \Pi \rightarrow \Pi$, the associated Poincare map, and fixing the parameter values $a=0.27857, b=3, c=0.3$ and $d=0.05$.

- Using rigorous ODE solvers for the systems and variational equations (CAPD library of the CAPD group (Krakow))

[^4]
## ... and now some theorems (CAP)

## Theorem

For each $u^{j} \in\left\{p_{1}^{8}, p_{2}^{8}, p_{3}^{8}, p_{4}^{16}, q_{1}^{12}, q_{2}^{14}\right\}$ there is a unique periodic orbit $v$ for $P$ of the principal period $j$ in the ball $B\left(u^{j}, 10^{-8}\right)$ in the maximum norm. Moreover, the resulting periodic points close to $p_{i}^{j}$ have one-dimensional unstable manifold and those corresponding to $q_{i}^{j}$ have two-dimensional invariant manifold.

Proof Let us fix $u^{j} \in\left\{p_{1}^{8}, p_{2}^{8}, p_{3}^{8}, p_{4}^{16}, q_{1}^{12}, q_{2}^{14}\right\}$ and define $F: \Pi^{j} \rightarrow \Pi^{j}$ by

$$
F_{j}\left(v_{1}, v_{2}, \ldots, v_{j}\right)=\left(v_{1}-P\left(v_{j}\right), v_{2}-P\left(v_{1}\right), \ldots, v_{j}-P\left(v_{j-1}\right)\right) .
$$

Solutions to $F_{j}\left(v_{1}, v_{2}, \ldots, v_{j}\right)=0$ correspond to $j$-periodic orbits for $P$ provided $v_{i} \neq v_{c}$ for $i \neq c$.
Put

$$
z_{0}=\left(v_{1}, v_{2}, \ldots, v_{j}\right)=\left(u^{j}, \hat{P}\left(u^{j}\right), \hat{P}^{2}\left(u^{j}\right), \ldots, \hat{P}^{j-1}\left(u^{j}\right)\right),
$$

where by $\hat{P}(u)$ we denote an approximate value of $P(u)$ obtained by nonrigorous numerical method.
Let $Z=B\left(z_{0}, 10^{-8}\right)$ be the ball centered at $z_{0}$ in the maximum norm. Using rigorous solvers for ODEs and variational equations from the CAPD library we computed the interval Newton operator

$$
N\left(F_{j}, Z, z_{0}\right)=z_{0}-\left[D F_{j}(Z)\right]^{-1} \cdot F_{j}\left(z_{0}\right)
$$

and obtained that $N\left(F_{j}, Z, z_{0}\right) \subset \operatorname{int}(Z)$. This proves that $F_{j}$ has unique zero $\left(v_{1}, \ldots, v_{j}\right)$ in $Z$. Moreover, this zero belongs to $N\left(F_{j}, Z, z_{0}\right)$ which in most cases had diameter less than $10^{-9}$. From these estimation we could conclude that $u^{j}$ has principal period $j$.

## ... and now some theorems (CAP)

Then we computed rigorous bounds for $D P^{j}\left(v_{1}\right) \in D P^{j}\left(B\left(u^{j}, 10^{-10}\right)\right)$ and we could check the hyperbolicity type of $u^{j}$ by analysis of the spectrum of the obtained interval matrix. The actual bounds for eigenvalues $\left\{\lambda_{1}, \lambda_{2}, \lambda_{3}\right\}$ are the following

| orbit | $\lambda_{1}$ | $\lambda_{2}$ | $\lambda_{3}$ | return time |
| :---: | :---: | :---: | :---: | :---: |
| $p_{1}^{8}$ | $2.7_{4}^{6}$ | $-0.16_{4}^{6}$ | $[-1,1] \cdot 10^{-11}$ | $56.585531937_{00}^{57}$ |
| $p_{2}^{8}$ | $-3.9_{89}^{91}$ | $-0.54_{4}^{7}$ | $[-5,5] \cdot 10^{-12}$ | $56.59832252_{61}^{73}$ |
| $p_{3}^{8}$ | -1.98 | $0.36_{4}^{6}$ | $[-1,1] \cdot 10^{-11}$ | $56.593931_{89}^{91}$ |
| $p_{4}^{16}$ | $[-3.30,-2.96]$ | $[-0.05,0.26]+[-0.13,0.13] i$ | $113.1853_{59}^{61}$ |  |
| $q_{1}^{12}$ | $-22 .{ }_{28}^{31}$ | $-3 .{ }_{06}^{14}$ | $[-8,8] \cdot 10^{-11}$ | $85.0883812_{29}^{36}$ |
| $q_{2}^{14}$ | $-4.3_{39}^{47}+5 .{ }_{36}^{48} i$ | $-4 .{ }_{39}^{47}-5 .{ }_{36}^{48} i$ | $[-5,5] \cdot 10^{-11}$ | $99.2973738_{34}^{53}$ |

## ... and now some theorems (CAP)

We have also proved that:

- there is an explicitly given trapping region $B \subset \Pi$ for $P$, i.e. $P(B) \subset B$,
- the maximal invariant set $A=\operatorname{inv}(P, B)$ contains three invariant sets, say $S_{1}, S_{2}, S_{3}$, on which the dynamics is $\Sigma_{2}$ chaotic, i.e. it is semiconjugated to the Bernoulli shift on two symbols,
- $S_{1}$ is hyperchaotic set with two positive Lyapunov exponents,
- $S_{2}$ and $S_{3}$ are chaotic sets with one positive Lyapunov exponent,
- there is a countable infinity of heteroclinic connections linking $S_{1}$ with $S_{2}, S_{2}$ with $S_{3}$ and $S_{1}$ with $S_{3}$,
- there is countable infinity of periodic orbits and heteroclinic/homoclinic orbits inside each horseshoe.


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## References

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## The Lorenz model

## The Lorenz model

$$
\frac{d x}{d t}=-\sigma x+\sigma y, \quad \frac{d y}{d t}=-x z+r x-y, \quad \frac{d z}{d t}=x y-b z
$$

Three dimensionless control parameters:

- $\sigma$ Prandtl number,
- b a positive constant,
- $r$ relative Rayleigh number.

The Saltzman values: $\sigma=10, b=8 / 3, r=28$


## The Lorenz model: Three-parametric analysis



## Theorem

For a given fixed $r>1$ the region where chaos is possible is bounded in $b$, and if $b \geq \epsilon>0$ then the region is bounded in $\sigma$ too. To be precise, outside a bounded region every positive semiorbit of the Lorenz system converges to an equilibrium.

## The Lorenz model: bifurcation analysis


(L.P. Shilnikov, 1980)

## The Lorenz model: but that's all?

## More T-points: the Lorenz model

Location of T-points in the Lorenz system is a quite complex task. And, what about locating all the T-points automatically?

In this case, the T-points are a kind of codimension-two heteroclinic loop. It connects a homoclinic curve with another spiral homoclinic curve.


## The Lorenz model: T-points

A new computer technique: more and more T-points


time

## The Lorenz model: T-points

A new computer technique: more and more T-points
Kneading sequence $\left\{\kappa_{n}\left(O^{+}\right)\right\}$defined (Milnor and Thurston, 1980)

$$
\kappa_{n}\left(O^{+}\right)=\left\{\begin{array}{cl}
+1, & \text { if } T^{n}\left(O^{+}\right)>0 \\
-1, & \text { if } T^{n}\left(O^{+}\right)<0 \\
0, & \text { if } T^{n}\left(O^{+}\right)=0
\end{array}\right.
$$

here $T^{n}\left(O^{+}\right)$is the $n$-th iterate of the right separatrix $O^{+}$of the origin. The condition $T^{n}\left(O^{+}\right)=0$ is interpreted as a homoclinic loop, i.e. the separatrix returns to the origin after $n$ steps.



The kneading invariant for the separatrix is defined in the form of a formal



## The Shimizu-Morioka model



Fig. 13. The $(\alpha, \lambda)$ bifurcation diagram for $B=0$.


## The Shimizu-Morioka model



## The Shimizu-Morioka model



Figure 2: Sketch of a partial bifurcation unfolding of a Bykov T-point (from [Bykov, 1980]) corresponding to a codimensiontwo heteroclinic connection between a saddle of the (2,1)-type and a saddle-focus of the (1,2)-type. It features the characteristic spirals corresponding to homoclinic bifurcations of the saddle. Turning points (labeled by M's) on the spiral are codimensiontwo points of inclination-switch bifurcations giving rise to stable periodic orbits through saddle-node and period-doubling bifurcations ( $l_{m}$-curves) and subsequent spiral structures of smaller scales between spiral's scrolls.

## The Shimizu-Morioka model: more and more T-points



## The Shimizu-Morioka model: fractal structure (Bykov)



## The Shimizu-Morioka model



## The Shimizu-Morioka model



## The Shimizu-Morioka model

- Fractal structure: our "open-air" homoclinic mines




[^0]:    *A. Abad, R. Barrio, F. Blesa and M. Rodriguez, "Algorithm 924: TIDES, a Taylor series Integrator for Differential EquationS," ACM Trans. Math. Software, Volume 39(1), 2012

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[^3]:    ${ }^{\S}$ P. Rech, Chaos and hyperchaos in a Hopfield neural network, Neurocomputing, 2011.

[^4]:    "Free-software: http://http://capd.ii.uj.edu.pl/

