Automatic differentiation, chaos indicators and dynamics

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Workshop on Stability and Instability in Mechanical Systems:
Applications and Numerical Tools
Barcelona, December 1 to 5, 2008

Summary

- Numerical study of dynamical systems

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Summary

1. Taylor's method: Automatic differentiation
2. Chaos Indicators
3. Open Hamiltonians: Hénon-Heiles Hamiltonian
4. Dissipative systems: The Lorenz model

Numerical requirements

1. Periodic orbits, invariant tori → Short integration times, sometimes with very high precision and simultaneous solution of the variational equations
2. Stability of the systems → Medium to large integration times and simultaneous solution of the variational equations

▶ TAYLOR's method: Automatic differentiation

$$\mathbf{y}(t_0) = \mathbf{y}_0,$$

$$\mathbf{y}(t_i) \simeq \mathbf{y}_i = \mathbf{y}_{i-1} + \frac{d\mathbf{y}(t_{i-1})}{dt} h_i + \frac{1}{2!}\frac{d^2\mathbf{y}(t_{i-1})}{dt^2} h_i^2 + \ldots + \frac{1}{p!}\frac{d^p\mathbf{y}(t_{i-1})}{dt^p} h_i^p .$$

- Very "new" ⟶ EULER
- **In Dynamical Systems** ⟶ NEW LIFE
  - Carles Simó and collaborators
    A. Jorba and M. Zou — TAYLOR
  - John Guckenheimer and collaborators
  - Willy Goovaerts and collaborators — MATCONT
  - GME (Zaragoza)

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Automatic differentiation

- But ... derivatives of the second member of the differential system

For ODEs ($\mathbf{y}'(t) = \mathbf{f}(t, \mathbf{y}(t))$):

$$\begin{aligned}\mathbf{y}'(t) &= \mathbf{f}(t, \mathbf{y}(t))\\ \mathbf{y}''(t) &= \mathbf{f}_t(t, \mathbf{y}(t)) + \mathbf{f}_{\mathbf{y}}(t, \mathbf{y}(t)) \cdot \mathbf{y}'(t)\\ \mathbf{y}'''(t) &= \mathbf{f}_{tt}(t, \mathbf{y}(t)) + \ldots\end{aligned}$$

  - The "drawback" in most classical books
  - Symbolic processors NO
  - Numerical differentiation NO
  - Automatic differentiation techniques
    - Exact (up to rounding errors) Taylor coefficients
    - Easy to implement
- Multiple precision libraries
  - mpfun and mpf90 (Prof. D. H. Bailey *et al.*)
  - gmp (GNU library in C)
- Interval arithmetic libraries
  - INTLIB, INTLAB, ...

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Automatic differentiation

Proposition (Moore (1966)): If $f, g, h : t \in \mathbb{R} \mapsto \mathbb{R}$ are functions $\mathcal{C}^n$ and denoting $a^{[j]}(t) = \dfrac{1}{j!}\, a^{(j)}(t)$, we have

- If $h(t) = f(t) \pm g(t)$ then $h^{[n]}(t) = f^{[n]}(t) \pm g^{[n]}(t)$
- If $h(t) = f(t) \cdot g(t)$ then $h^{[n]}(t) = \sum_{i=0}^{n} f^{[n-i]}(t)\, g^{[i]}(t)$
- If $h(t) = f(t)/g(t)$ then $h^{[n]}(t) = \frac{1}{g^{[0]}(t)} \left\{ f^{[n]}(t) - \sum_{i=1}^{n} h^{[n-i]}(t)\, g^{[i]}(t) \right\}$
- If $h(t) = f(t)^{\alpha}$ then
  $h^{[0]}(t) = (f^{[0]}(t))^{\alpha}, \quad h^{[n]}(t) = \dfrac{1}{n\, f^{[0]}(t)} \sum_{i=0}^{n-1} (n\,\alpha - i(\alpha+1))\, f^{[n-i]}(t)\, h^{[i]}(t)$
- If $h(t) = \exp(f(t))$ then
  $h^{[0]}(t) = \exp\left(f^{[0]}(t)\right), \quad h^{[n]}(t) = \frac{1}{n} \sum_{i=0}^{n-1} (n-i)\, f^{[n-i]}(t)\, h^{[i]}(t)$
- If $h(t) = \ln(f(t))$ then
  $h^{[0]}(t) = \ln\left(f^{[0]}(t)\right), \quad h^{[n]}(t) = \frac{1}{f^{[0]}(t)} \left\{ f^{[n]}(t) - \dfrac{1}{n} \sum_{i=1}^{n-1} (n-i)\, h^{[n-i]}(t)\, f^{[i]}(t) \right\}$
- If $g(t) = \cos(f(t))$ and $h(t) = \sin(f(t))$ then

$$g^{[0]}(t) = \cos\left(f^{[0]}(t)\right), \quad g^{[n]}(t) = -\frac{1}{n} \sum_{i=1}^{n} i\, h^{[n-i]}(t)\, f^{[i]}(t)$$
$$h^{[0]}(t) = \sin\left(f^{[0]}(t)\right), \quad h^{[n]}(t) = \frac{1}{n} \sum_{i=1}^{n} i\, g^{[n-i]}(t)\, f^{[i]}(t)$$

Implementation details

- Variable Stepsize[1]
  - Combination of estimates of Lagrange remainder and Newton method

$$h = h_0 - \frac{h_0^{n-1}\,(A + h_0\,B) - \texttt{Tol}}{h_0^{n}\,\big((n-1)\,A + h_0\,n\,B\big)}.$$

with $\texttt{Tol} = \min\Big\{\texttt{TolRel}\cdot\max\{\|\mathbf{y}^{[0]}(t_i)\|_\infty,\ \|\mathbf{y}^{[1]}(t_i)\|_\infty\},\ \texttt{TolAbs}\Big\}$ and

$$A = \|\mathbf{y}^{[n-1]}(t_i)\|_\infty, \qquad B = n\,\|\mathbf{y}^{[n]}(t_i)\|_\infty$$

  - Information of last two coefficients (embedded methods)

$$h = \texttt{fac}\cdot\min\left\{\left(\frac{\texttt{Tol}}{\|\mathbf{y}^{[n-1]}(t_i)\|_\infty}\right)^{1/(n-1)},\ \left(\frac{\texttt{Tol}}{\|\mathbf{y}^{[n]}(t_i)\|_\infty}\right)^{1/n}\right\}$$

  - Defect error control (possible rejected stepsizes, no rejected steps)

$$\text{if}\quad \|\mathbf{y}'_{i+1} - \mathbf{f}(t_{i+1},\,\mathbf{y}_{i+1})\|_\infty > \texttt{Tol}\quad\text{then}\quad \widetilde{h}_{i+1} = \texttt{facr}\cdot h_{i+1},$$

[1] R. Barrio, Appl. Math. Comput. 163 (2005) 525–545.

Implementation details

- Variable Order[2]

if $i = \dot{M}$ **then**

$n_{i+1} = n_i$

$h_{\max} = \max\{ h_{i-M}, \ldots, h_{i-1} \}, \quad h_{\min} = \min\{ h_{i-M}, \ldots, h_{i-1} \}$

if $((h_{i-M} < h_{\min})\ \texttt{.or.}\ (h_{i-M} = h_{\min}\ \texttt{.and.}\ n_{i-1} > n_i))$ **then**

$$h_{\text{est}}^{-} = \texttt{tol}^{1/(n_i - p + 1)} \cdot \|\mathbf{Y}_{n_i - p}\|_{\infty}^{-1/(n_i - p)}$$

if $\left(\dfrac{n_i - p + 1}{n_i + 1}\right)^2 < \texttt{fac1} \cdot \dfrac{h_{\text{est}}^{-}}{h_i}$ **then**

$n_{i+1} = n_i - p$

end if

else if $((h_{i-M} > h_{\max})\ \texttt{.or.}\ (h_{i-M} = h_{\max}\ \texttt{.and.}\ n_{i-1} < n_i))$ **then**

$$\rho_{\text{est}} = \min\left\{ \left\| \frac{\mathbf{Y}_{n_i - 1}}{\mathbf{Y}_{n_i}} \right\|_{\infty}, \left\| \frac{\mathbf{Y}_{n_i - 2}}{\mathbf{Y}_{n_i}} \right\|_{\infty}^{1/2}, \left\| \frac{\mathbf{Y}_{n_i - 3}}{\mathbf{Y}_{n_i - 1}} \right\|_{\infty}^{1/2} \right\}$$

$$h_{\text{est}}^{+} = \texttt{tol}^{1/(n_i + p + 1)} \cdot \left(\frac{\|\mathbf{Y}_{n_i}\|_{\infty}}{\rho_{\text{est}}^{p}} \right)^{-1/(n_i + p)}$$

if $\left(\dfrac{n_i + p + 1}{n_i + 1}\right)^2 < \texttt{fac2} \cdot \dfrac{h_{\text{est}}^{+}}{h_i}$ **then**

$n_{i+1} = n_i + p$

end if

end if

else

$n_{i+1} = n_i$

end if

---

[2] R. Barrio, F. Blesa and M. Lara, Comput. Math. Appl. 50 (1-2) (2005) 93–111.

Advantages/Disadvantages

- Advantages
  - Dense output $\rightarrow$ Poincaré Surfaces of Section
  - Good stability properties[3] (for an explicit method)
  - Versatile (ODEs, DAEs, BVPs,...)
  - Direct solution of variational equations $\rightarrow$ Extended Taylor method[4]

$$\mathbf{y}' = \mathbf{f}(t, \mathbf{y}; \mathbf{p}), \qquad \mathbf{s}_k' = \frac{\partial \mathbf{f}}{\partial \mathbf{y}} \cdot \mathbf{s}_k + \frac{\partial \mathbf{f}}{\partial p_k}, \qquad \mathbf{s}_k'' =$$

    Interval methods: Berz *et al.*, Zgliczynski and Wilczak
  - Methods of any order: arbitrary precision
  - Variable stepsize and order[5]
  - Basic in Computer Aided Proofs (Lohner's algorithm).
    see just next talk: Zgliczynski
- Disadvantages
  - *Stiff* problems
  - ?

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Proposition

[a] *If* $f(t, \mathbf{y}(t)), g(t, \mathbf{y}(t)) : (t, \mathbf{y}) \in \mathbb{R}^{s+1} \mapsto \mathbb{R}$ *functions of class* $\mathcal{C}^n$, $\mathbf{i} = (i_1, \ldots i_s) \in \mathbb{N}_0^s$, $\mathbf{i}^* = \mathbf{i} - (0, \ldots, 0, 1, 0, \ldots, 0) = (i_1, i_2, \ldots, i_k - 1, 0, \ldots, 0)$ *and* $\|\mathbf{i}\| = \sum_{j=1}^{s} i_j$ *the total order of derivation, we denote*

$$f^{[j,\,\mathbf{i}]} := \frac{1}{j!}\,\frac{\partial^{\|\mathbf{i}\|} f^{(j)}(t)}{\partial y_1^{i_1}\,\partial y_2^{i_2}\cdots\partial y_s^{i_s}}, \qquad f^{[j,\,\mathbf{0}]} := f^{[j]} = \frac{1}{j!}\,\frac{d^j f(t)}{dt^j},$$

the j*th Taylor coefficient of the partial derivative of* $f(t, \mathbf{y}(t))$ *with respect to* $\mathbf{i}$ *and*

$$\widetilde{h}_{n,\,\mathbf{i}}^{[j,\,\mathbf{v}]} = h^{[j,\,\mathbf{v}]}, \quad (j \neq n \text{ or } \mathbf{v} \neq \mathbf{i}), \qquad \widetilde{h}_{n,\,\mathbf{i}}^{[n,\,\mathbf{i}]} = 0.$$

Besides, given $\mathbf{v} = (v_1, \ldots, v_s) \in \mathbb{N}_0^s$ *we define the multi-combinatorial number* $\binom{\mathbf{i}}{\mathbf{v}} = \binom{i_1}{v_1} \cdot \binom{i_2}{v_2} \cdots \binom{i_s}{v_s}$, *and we consider the classical partial order in* $\mathbb{N}_0^s$. *Then*

(v) *If* $h(t) = f(t)^\alpha$ *with* $\alpha \in \mathbb{R}$ *then* $h^{[0,\,\mathbf{0}]} = (f^{[0]}(t))^\alpha$ *and*

$$h^{[0,\,\mathbf{i}]} = \frac{1}{f^{[0]}} \sum_{\mathbf{v} \leq \mathbf{i}^*} \binom{\mathbf{i}^*}{\mathbf{v}} \left\{ \alpha\, h^{[0,\,\mathbf{v}]} \cdot f^{[0,\,\mathbf{i}-\mathbf{v}]} - \widetilde{h}_{0,\,\mathbf{i}}^{[0,\,\mathbf{i}-\mathbf{v}]} \cdot f^{[0,\,\mathbf{v}]} \right\}, \qquad \mathbf{i} > \mathbf{0},$$

$$h^{[n,\,\mathbf{i}]} = \frac{1}{n\, f^{[0]}} \sum_{j=0}^{n} (n\,\alpha - j(\alpha+1)) \left\{ \sum_{\mathbf{v} \leq \mathbf{i}} \binom{\mathbf{i}}{\mathbf{v}} \widetilde{h}_{n,\,\mathbf{i}}^{[j,\,\mathbf{v}]} \cdot f^{[n-j,\,\mathbf{i}-\mathbf{v}]} \right\}, \quad n > 0,\ \mathbf{i} > \mathbf{0}.$$

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Computational complexity

Proposition

If the evaluation of $f(t, \mathbf{y}(t))$ *involves* k *elementary functions* ($\times$, $/$, ln, exp, sin, cos, $\ldots$) *then the computational complexity of the evaluation of* $f^{[0]}, f^{[1]}, \ldots, f^{[n-1]}$ *is* $k\, n^2 + \mathcal{O}(n)$. *(In the case of linear functions* $k\, n + \mathcal{O}(1)$*)*

Proposition

If the evaluation of $f(t, \mathbf{y}(t))$ *involves* k *elementary functions* ($\times$, $/$, ln, exp, sin, cos, $\ldots$) *and given* $\mathbf{i} = (i_1, i_2, \ldots, i_s) \in \mathbb{N}_0^s$ *then the computational complexity of the evaluation of* $f^{[0,\,\mathbf{i}]}, f^{[1,\,\mathbf{i}]}, \ldots, f^{[n-1,\,\mathbf{i}]}$*, supposing already known all the derivatives of index* $\mathbf{v} < \mathbf{i}$*, is*

$$\mathcal{O}\left(\prod_{j=1}^{s} (i_j + 1) \cdot k\, n^2\right).$$

Corollary

The computational complexity of evaluating the Taylor coefficients of a partial derivative of f *is twice the complexity of evaluating the Taylor coefficients of* f*, and the computational complexity of evaluating the Taylor coefficients of a second order partial*

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The computational complexity of evaluating the Taylor coefficients of a partial derivative of f *is twice the complexity of evaluating the Taylor coefficients of* f*, and the computational complexity of evaluating the Taylor coefficients of a second order partial derivative of* f *is, once the coefficients of the first order partial derivatives are known, four times the complexity of evaluating the Taylor coefficients of* f *in the case of* $\partial^2 f / \partial y_i\, \partial y_j$ $(i \neq j)$ *and three times in the case* $\partial^2 f / \partial y_i^2$.

Programming

Two body problem (Kepler)

$$\ddot{x} = -\frac{x}{(x^2+y^2)^{3/2}}, \qquad \ddot{y} = -\frac{y}{(x^2+y^2)^{3/2}}$$

KEPLER PROBLEM

for $m = 0$ to $n-2$ do

$$c = (1+m)(2+m)$$

$$s_1^{[m]} = \boxed{x \times x}^{[m]} + \boxed{y \times y}^{[m]}$$

$$s_2^{[m]} = \boxed{(s_1)^{-3/2}}^{[m]}$$

$$x^{[m+2]} = -\boxed{x \times s_2}^{[m]}/c$$

$$y^{[m+2]} = -\boxed{y \times s_2}^{[m]}/c$$

end

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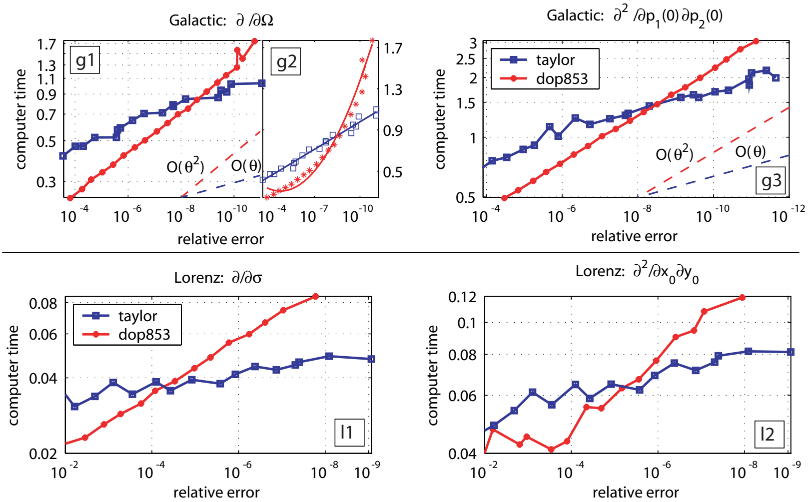
\quad y^{[m+2]} = -\boxed{y \times s_2}^{[m]}/c \\
\texttt{end}
\end{array}
$$

KEPLER PROBLEM & SENSITIVITY VALUES

$$
\begin{array}{l}
\texttt{for} \quad m=0 \quad \texttt{to} \quad n-2 \quad \texttt{do} \\
\quad c = (1+m)(2+m) \\
\quad \texttt{for} \quad \mathbf{v}=\mathbf{0} \quad \texttt{to} \quad \mathbf{i} \quad \texttt{do} \\
\qquad s_1^{[m,\mathbf{v}]} = \boxed{x \times x}^{[m,\mathbf{v}]} + \boxed{y \times y}^{[m,\mathbf{v}]} \\
\qquad s_2^{[m,\mathbf{v}]} = \boxed{(s_1)^{-3/2}}^{[m,\mathbf{v}]} \\
\qquad x^{[m+2,\mathbf{v}]} = -\boxed{x \times s_2}^{[m,\mathbf{v}]}/c \\
\qquad y^{[m+2,\mathbf{v}]} = -\boxed{y \times s_2}^{[m,\mathbf{v}]}/c \\
\quad \texttt{end} \\
\texttt{end}
\end{array}
$$

• Numerical test: Taylor series method vs. DOP853 (Hairer & Wanner)



For high-precision demands Taylor series method seems to be the fastest method for smooth low-dimension problems (non-stiff)

Summary

Chaos indicators

Techniques to *detect* chaos (not to proof chaos).

- Poincaré Surfaces of Section
  (Poincaré, Birkhoff, Hénon & Heiles (1964))
  - 2DOF
  - In some cases it is impossible to obtain a transverse section for the whole flow (Dullin & Wittek '95)

- Maximum Lyapunov Exponent (MLE)

$$\frac{d\boldsymbol{y}}{dt} = \boldsymbol{f}(t, \boldsymbol{y}), \qquad \boldsymbol{y}(0) = \boldsymbol{y}_0,$$
$$\frac{d\delta\boldsymbol{y}}{dt} = \frac{\partial \boldsymbol{f}(t, \boldsymbol{y})}{\partial \boldsymbol{y}} \delta\boldsymbol{y}, \quad \delta\boldsymbol{y}(0) = \delta\boldsymbol{y}_0$$

  is given by $\mathrm{MLE} = \lim_{t \to +\infty} \frac{1}{t} \ln \frac{\|\delta\boldsymbol{y}(t)\|}{\|\delta\boldsymbol{y}(0)\|}$
  - MLE gives a way of measuring the degree of sensitivity to initial conditions
  - A limit in the definition $\longrightarrow$ long time integration

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is given by $\mathrm{MLE} = \lim_{t\to+\infty} \frac{1}{t} \ln \frac{\|\delta\boldsymbol{y}(t)\|}{\|\delta\boldsymbol{y}(0)\|}$

  - MLE gives a way of measuring the degree of sensitivity to initial conditions
  - A limit in the definition $\longrightarrow$ long time integration

Fast Chaos indicators

- Fast techniques to *detect* chaos.
- Classification:
  - Variational methods Use the variational equations:

    Heliticity and Twist Angles (Contopoulos & Voglis), Smaller ALigment Index (SALI) (Skokos), Mean Exponential Growth factor of Nearby Orbits (MEGNO) (Cincotta & Simó), Fast Lyapunov Indicator (FLI) (Froeschlé & Lega), $\mathrm{OFLI}_{\mathrm{TT}}^{2}$ or OFLI2 (Barrio).
  - Time series methods Analyse the spectrum of some scalar function of a single orbit:

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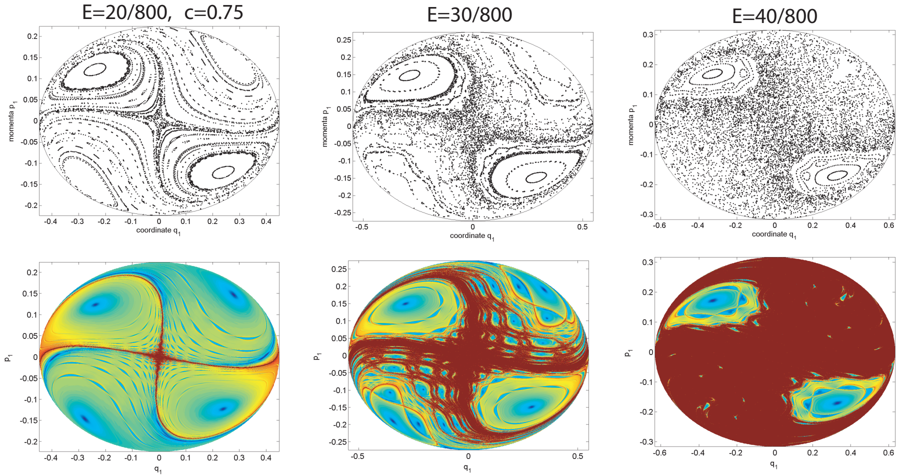
Extensible-Pendulum

$$\mathcal{H}(q_1, q_2, p_1, p_2) = \frac{1}{2}(p_1^2 + p_2^2) + \frac{1}{2}((1-c)\,q_1^2 + q_2^2 - c\,q_1^2\,q_2),$$



Variational methods

- Mean Exponential Growth factor of Nearby Orbits (MEGNO) (Cincotta & Simó), based on the integral form of the MLE

$$Y(t) = \frac{2}{t}\int_{t_0}^{t} \frac{\dot{\delta}(\hat{t})}{\delta(\hat{t})}\,\hat{t}\,\mathrm{d}\hat{t}, \quad \bar{Y}(t) = \frac{1}{t}\int_{t_0}^{t} Y(\hat{t})\mathrm{d}\hat{t}, \quad (\delta(t) = \|\delta \boldsymbol{y}(t)\|)$$

  - $\lim \bar{Y}(t) = 0$ for harmonic oscillations, 2 for ordered motion, asymptotically $\bar{Y}(t) \approx t \cdot \mathrm{MLE}/2$ for chaotic orbits.
  - “Absolute" information
- Fast Lyapunov Indicator (FLI) (OFLI) (Froeschlé & Lega)

$$\begin{aligned} \mathrm{FLI}(\boldsymbol{y}(0), \delta\boldsymbol{y}(0), t_f) &= \sup_{0<t<t_f} \log \|\delta \boldsymbol{y}(t)\| \\ \mathrm{OFLI}(\boldsymbol{y}(0), \delta\boldsymbol{y}(0), t_f) &= \sup_{0<t<t_f} \log \|\delta \boldsymbol{y}^{\perp}(t)\| \end{aligned}$$

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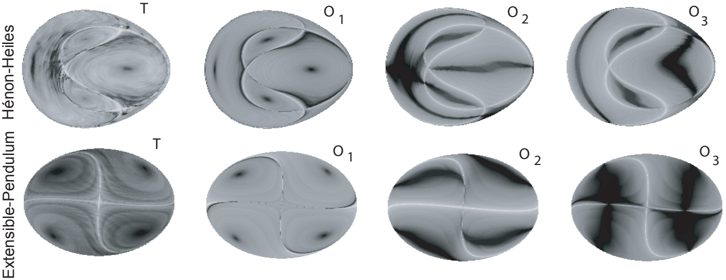
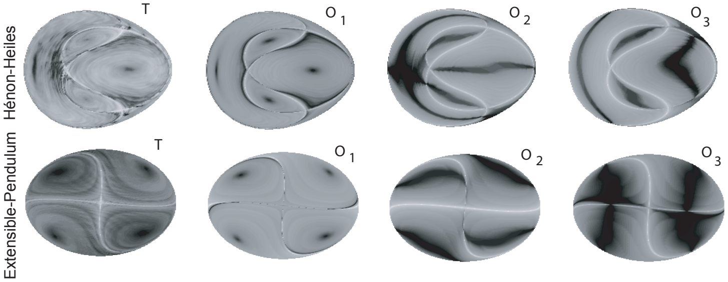

Hénon-Heiles
Extensible-Pendulum
T
O 1
O 2
O 3
T
O 1
O 2
O 3


Hénon-Heiles
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O 1
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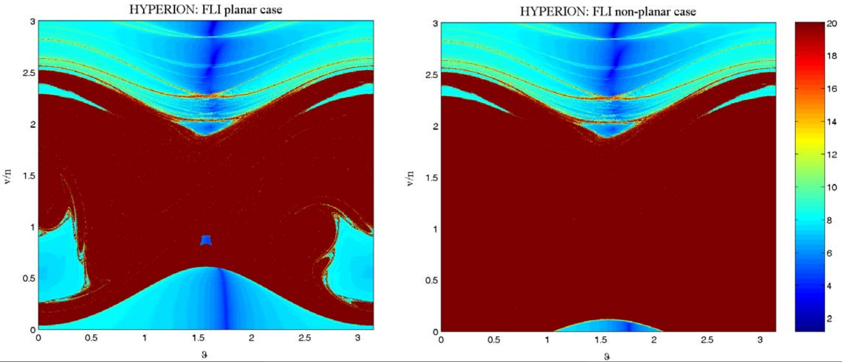
HYPERION: FLI planar case
HYPERION: FLI non-planar case
ν/n
ϑ

How to choose the initial conditions?

- OFLI2[6] Chaos Indicator

$$\mathrm{OFLI2} := \sup_{0<t<t_f} \log \|\{\delta \mathbf{y}(t) + \frac{1}{2}\,\delta^2 \mathbf{y}(t)\}^{\perp}\|,$$

where $\delta \mathbf{y}$ and $\delta^2 \mathbf{y}$ are the first and second order sensitivities with respect to carefully chosen initial vectors:

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[6] R. Barrio, Chaos Solitons Fractals 25 (3) (2005) 711–726.
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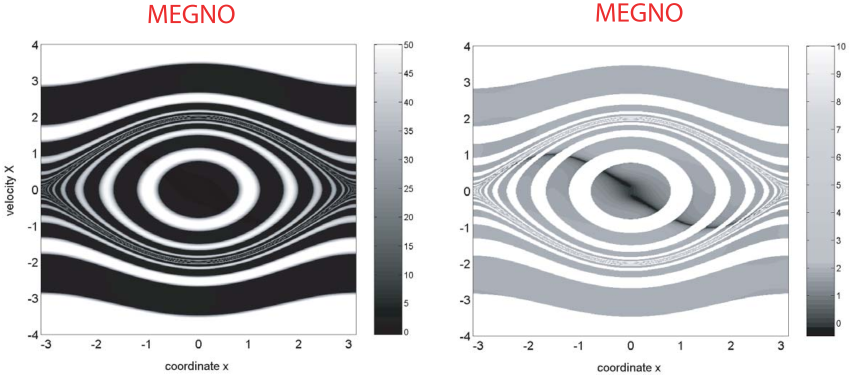
Coupled pendulum: case $y = Y = 0$.

Test Problem: A coupled pendulum system with two degrees of freedom.

$$\mathcal{H} = \frac{1}{2}\left(X^2 + Y^2\right) - (1 + a\,b)\,\cos x - a\cos y + a\,b\,\cos x \cos y.$$

The problem is integrable for all initial conditions when either a or b are equal 0.

- Using the 2DOF formulation and $\delta \boldsymbol{y}(0) = (1, 1, 1, 0)$



Resolving the contradiction: case $y = Y = 0$.

$$\delta\ddot{x} = -\cos x\,\delta x, \qquad \delta\ddot{y} = -a\,(1 - b\,\cos x)\,\delta y.$$

- Suppose that we are in the circulation regime and $\cos x \approx \cos \nu\, t$
- New independent variable $u = \nu\, t$, and a parameter $\omega^2 = a/\nu^2$

Standard form of the Mathieu equation: $\dfrac{d^2(\delta y)}{du^2} = -\omega^2\,(1 - b\cos u)\,\delta y$

known to be unstable if any of the parametric resonances $\omega \approx \frac{k}{2}, \quad k \in \mathbb{Z}_+$, occurs. The width of the "Arnold tongues" of instability increases with b but decreases with k.

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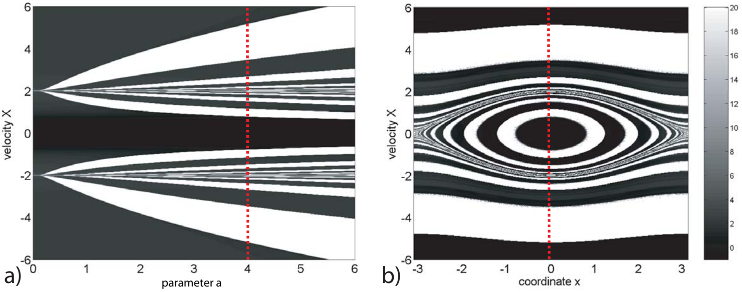
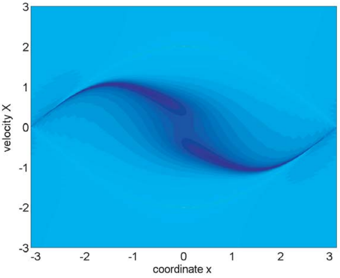
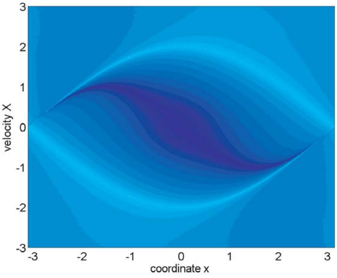


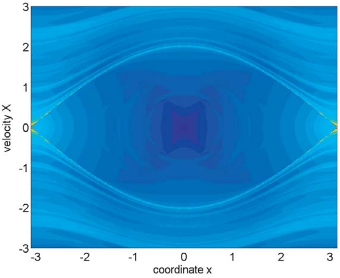
More spurious structures

MEGNO



FLI





OFLI2

Pendulum problem

$$\delta x(0) = \delta X(0) = 1$$

Why?

Proposición (Haken)

The function $V = \mathbf{f}(t, \rho)$ is the solution of the variational equation with initial conditions $\xi_0 = \mathbf{f}(t_0, \rho_0)$. Moreover, if the support of the ergodic measure p does not reduce to a fixed point then these initial conditions in the variational equations generate a zero Lyapunov exponent.

- For any orbit at least one Lyapunov exponent vanishes.
- Hamiltonian systems: At least two Lyapunov exponents are zero.
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Why?: Hamiltonian systems

- 1DOF Conservative Hamiltonians $\longrightarrow$ both Lyapunov exponents vanish
- The direction tangent to the flow generates a very low value of the variational Chaos Indicators because for periodic orbits the ratio $\|\boldsymbol{f}(t)\|/\|\boldsymbol{f}(t_0)\|$ has only small variations.
- In order to have an initial vector $\xi_0 = (\delta x_0, \delta y_0)^\top$ for the variational equations tangent to the flow in the pendulum equations for $\delta y_0 \neq 0$,

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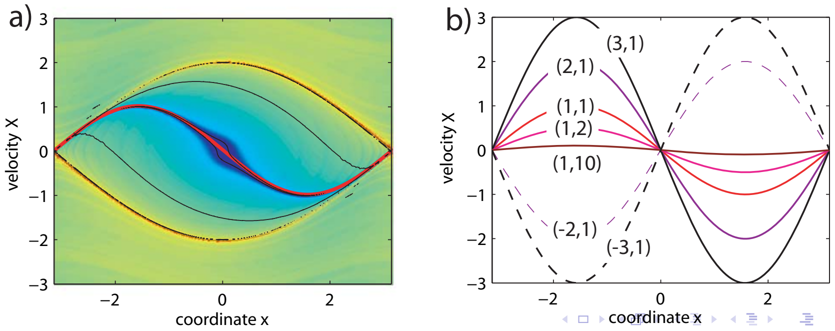

How to avoid the spurious structures?

- It seems reasonable to avoid the tangent direction.
- In 1DOF Hamiltonians: the vector orthogonal to the flow, $\nabla \mathcal{H}$.

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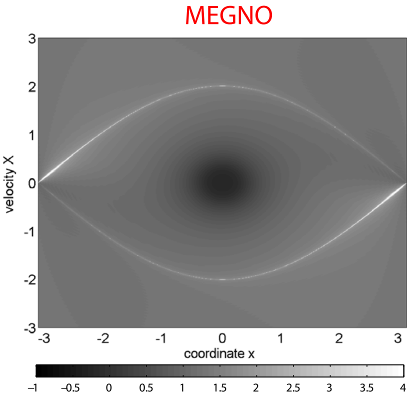
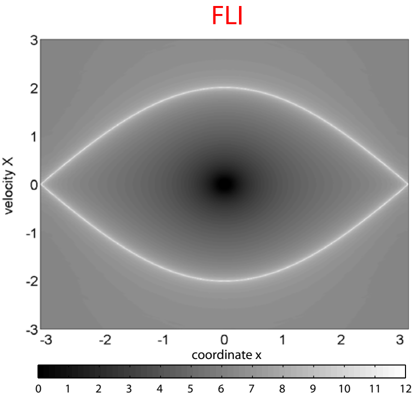
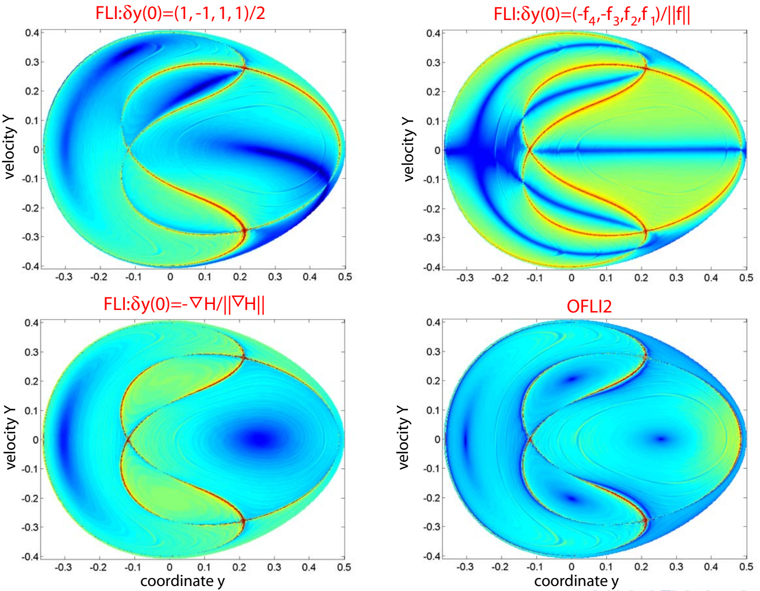




How to avoid the spurious structures? HH

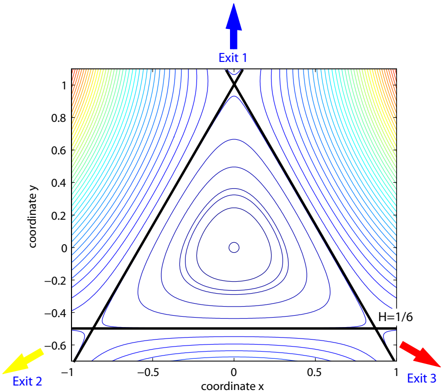


Summary

$$\mathcal{H} = \frac{1}{2}(X^2 + Y^2) + \frac{1}{2}(x^2 + y^2) + \left(x^2 y - \frac{1}{3}y^3\right)$$

Symmetries:

- the spatial group is a dihedral group D_3
- the complete symmetry group is $D_3 \times \mathcal{T}$ ($\mathcal{T}$ is a $\mathbb{Z}_2$ symmetry, *the time reversal symmetry*)



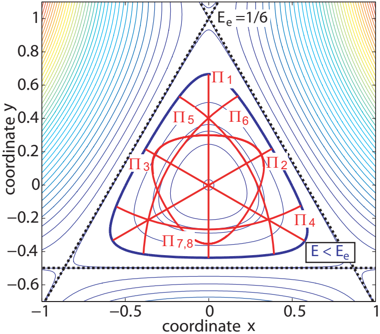
[7] R. Barrio, F. Blesa and S. Serrano, Europhysics Letters, 82, (2008) 10003.
R. Barrio, F. Blesa and S. Serrano, Preprint (2008).

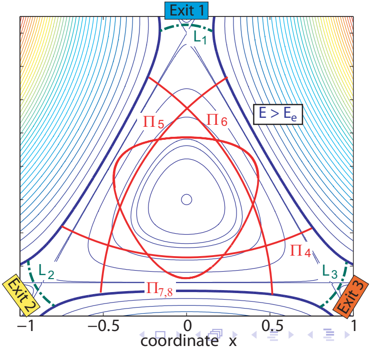
Theorem (Weinstein (1973))

If the Hamiltonian $\mathcal{H}(\mathbf{x},\mathbf{X})$ is of class $\mathcal{C}^2$ near $(\mathbf{x},\mathbf{X}) = (0,0)$, where $\mathbf{x},\mathbf{X} \in \mathbb{R}^n$, and the Hessian matrix $\mathcal{H}_{**}(0,0)$ is positive definite, then for ε sufficiently small any energy surface $\mathcal{H}(\mathbf{x},\mathbf{X}) = \mathcal{H}(0,0) + \varepsilon^2$ contains at least n periodic orbits of the corresponding Hamiltonian equations whose periods are close to those of the linear system $\dot{\mathbf{z}} = J\mathcal{H}_{**}(0,0)\mathbf{z}$.

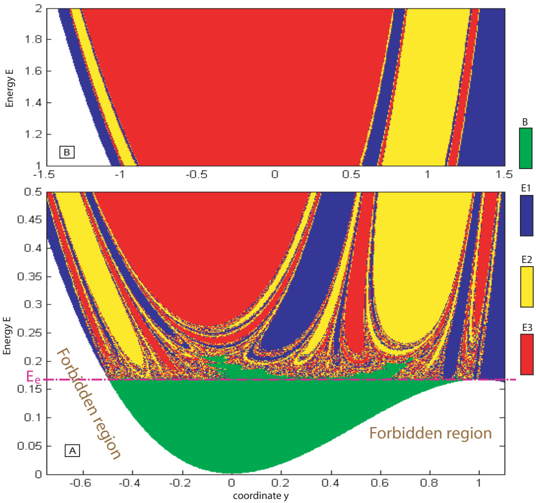
Nonlinear normal modes:

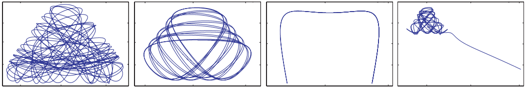
- from Weinstein's theorem ≥ 2
- from the symmetries 8: Π_i, $i = 1, \ldots, 8$ (Churchill *et al.* (1979))





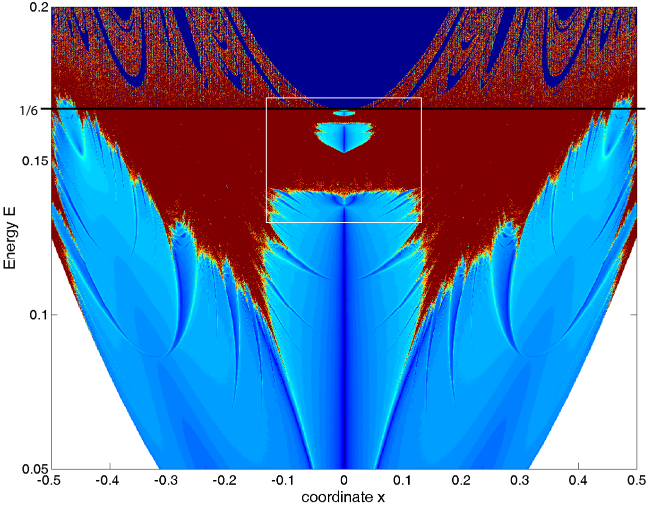
Escape basins: plane (y, E)





- for $\mathcal{H} < 1/6$ all orbits are bounded.
- for $1/6 < \mathcal{H} \lesssim 0.22$ most orbits are escape orbits and some KAM tori persist.
- for $0.22 \lesssim \mathcal{H}$ no KAM tori and all orbits are escape orbits **(?)**.

Fractal structures near the critical energy level: Π_1



Below escape energy:

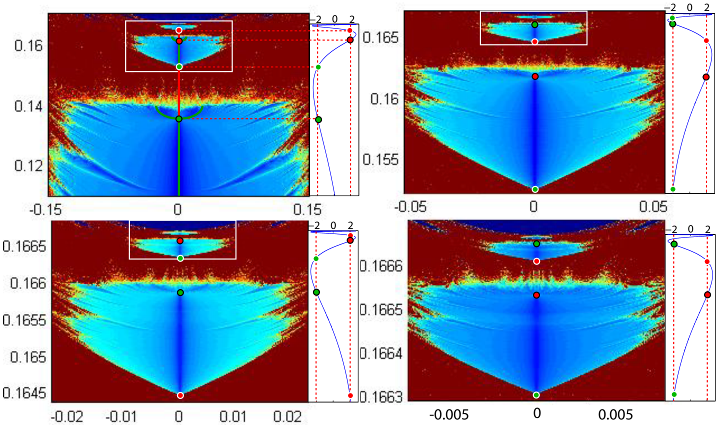
- blue regular
- red chaos.

Above escape energy:

- dark blue escape orbits.
- red escape with transient chaos.

- Π_1 stability varies as E approaches the critical value.

Fractal structures near the critical energy level



- The Π_1 (and Π_2 and Π_3) periodic orbit goes through an infinite sequence of transitions in stability type (Churchill *et al* (1980))
- Sequence of isochronous and period-doubling bifurcations. An infinite sequence of decreasing in size fractal regular regions (Barrio, Blesa and Serrano (2008))

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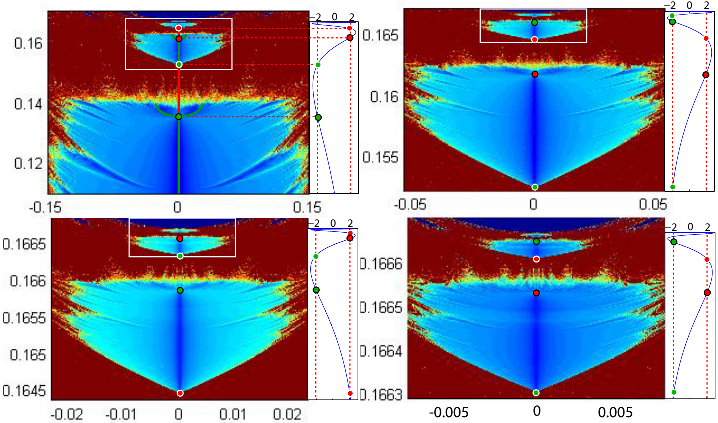

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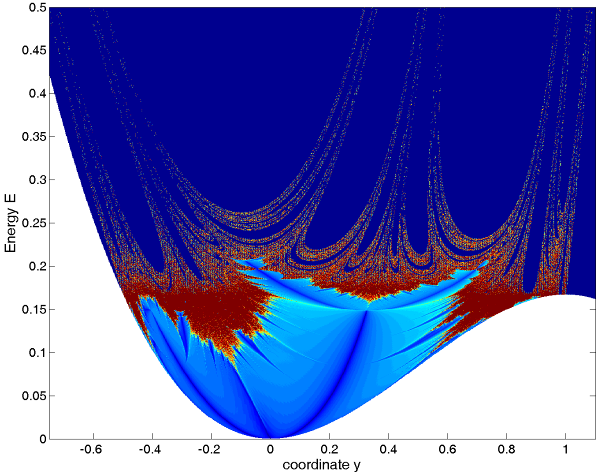
Fractal and regular bounded structures
In the KAM region

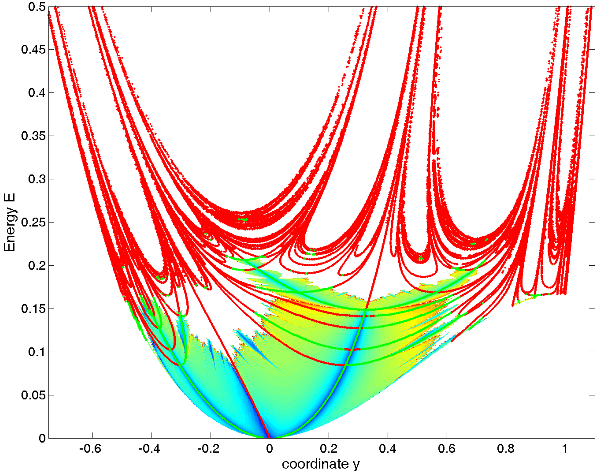


Above the escape energy:

- KAM tori disappear on y-axis around $E \approx 0.2113$.

Bounded regions far from the KAM tori?

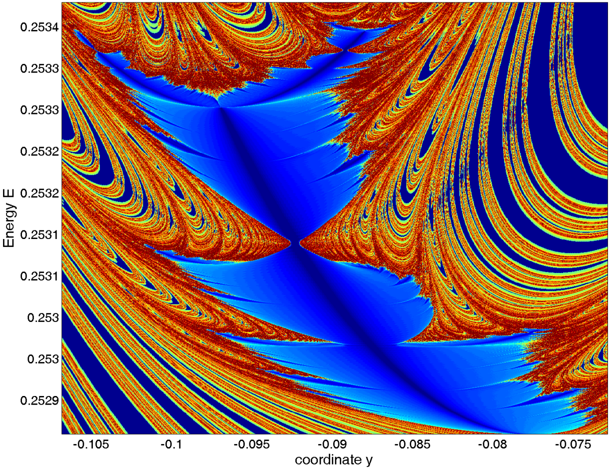
Symmetric Periodic Orbits



- ✓ Periodic orbits.
- ✓ OFLI2 chaos indicator.
- ✓ Red: unstable p.o.
- ✓ Green: stable p.o.
- ✓ Small zones of stable periodic orbits.

Fractal and regular bounded structures

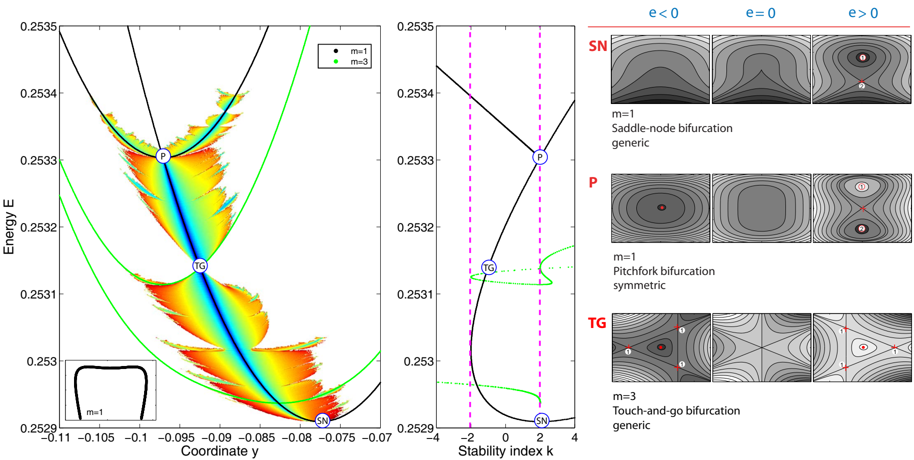
In the escape region



Above the escape energy:

- Small regular region around $E \approx 0.253$.
- Self-similar regions with chains of bifurcations inside.

Bifurcations



- Without D_3 symmetry.
- Stable and bounded regions far form the KAM tori

Summary

The Lorenz model[8]

The Lorenz model

$$\frac{dx}{dt} = -\sigma x + \sigma y, \quad \frac{dy}{dt} = -xz + r x - y, \quad \frac{dz}{dt} = xy - b z,$$

Three dimensionless control parameters:
σ Prandtl number, b a positive constant, r relative Rayleigh number.

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

- The fixed points:

$$C^0 = (0,0,0), \qquad C^{\pm} = (\pm\sqrt{b(r-1)}, \pm\sqrt{b(r-1)}, r-1) \quad \text{for } r > 1$$

[8] R. Barrio and S. Serrano, Physica D, 229, (2007) 43–51.
R. Barrio and S. Serrano, Preprint (2008).

Classical scheme

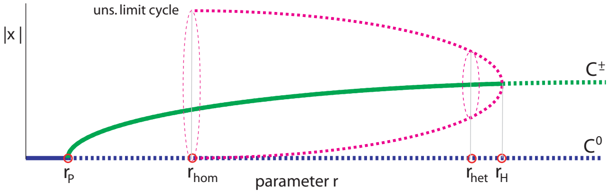
For $r < 1$, C^0 is globally attracting.

$r_{\mathrm{P}} = 1$ pitchfork bifurcation.

For $1 < r < r_{\mathrm{H}} \approx 24.74$. C^0 unstable and $C^{\pm}$ stable.

- For $1 < r < r_{\mathrm{hom}} \approx 13.926$ trajectories $\rightarrow$ equilibrium points.
- For $r_{\mathrm{hom}} < r < r_{\mathrm{het}} \approx 24.06$. Unst. limit cycles + transient chaos.
- For $r_{\mathrm{het}} < r < r_{\mathrm{H}}$. Unst. limit cycles + chaotic stable attractor.
- $r = r_{\mathrm{H}}$ subcritical Andronov-Hopf bifurcation.

For $r > r_{\mathrm{H}} \approx 24.74$. C^0 and $C^{\pm}$ unst. equilibrium points.



Classical scheme

For $r < 1$, C^0 is globally attracting.

$r_{\mathrm{P}} = 1$ pitchfork bifurcation.

For $1 < r < r_{\mathrm{H}} \approx 24.74$. C^0 unstable and $C^{\pm}$ stable.

- For $1 < r < r_{\mathrm{hom}} \approx 13.926$ trajectories $\rightarrow$ equilibrium points.
- For $r_{\mathrm{hom}} < r < r_{\mathrm{het}} \approx 24.06$. Unst. limit cycles + transient chaos.
- For $r_{\mathrm{het}} < r < r_{\mathrm{H}}$. Unst. limit cycles + chaotic stable attractor.
- $r = r_{\mathrm{H}}$ subcritical Andronov-Hopf bifurcation.

For $r > r_{\mathrm{H}} \approx 24.74$. C^0 and $C^{\pm}$ unst. equilibrium points.

Up to $r \sim 146$: large chaotic region

$r \sim 146$ to $r \sim 166.1$: regular region

Up to $r \sim 214$: chaotic region

Afterwards: regular region

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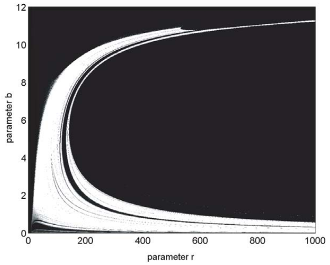
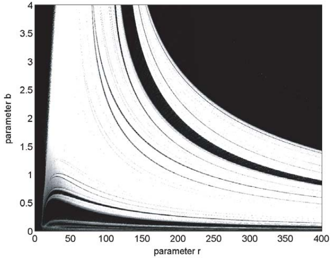
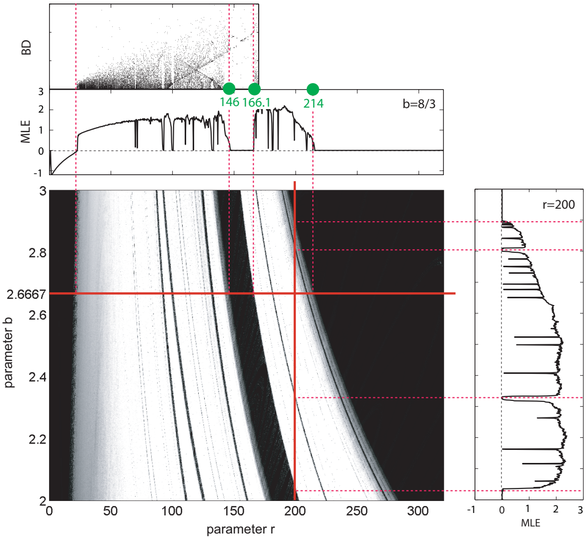
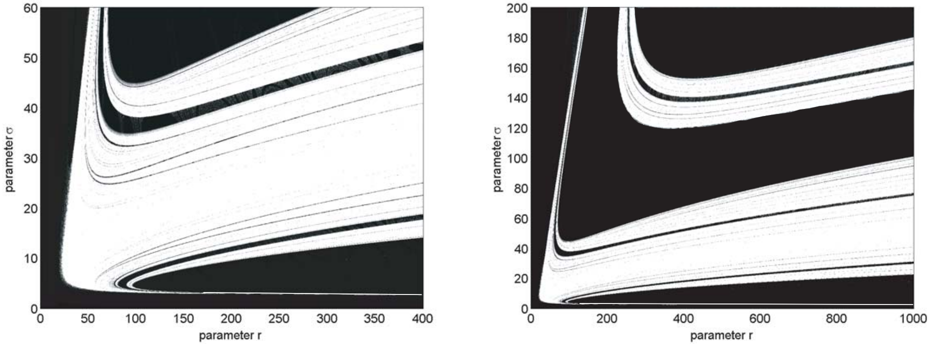
Biparametric analysis: $\sigma = 10$







Biparametric analysis: $b = 8/3$



Fractral estructures: Fat fractal exponent γ, $\mu(\varepsilon) = \mu_0 + K\,\varepsilon^\gamma$

$$\gamma = 0.3227(\pm 0.1336)$$

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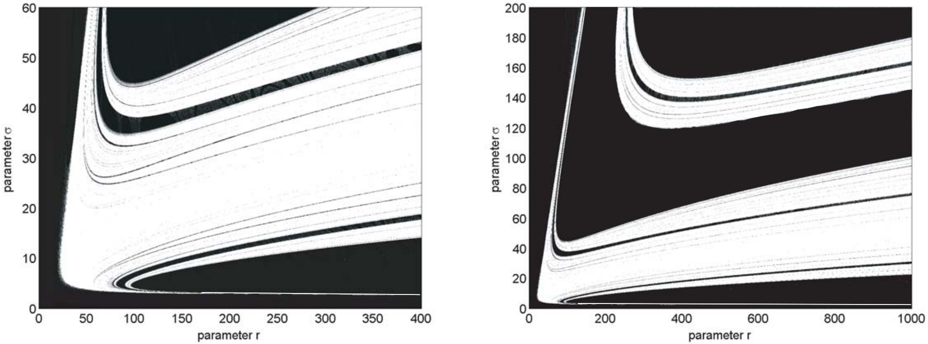

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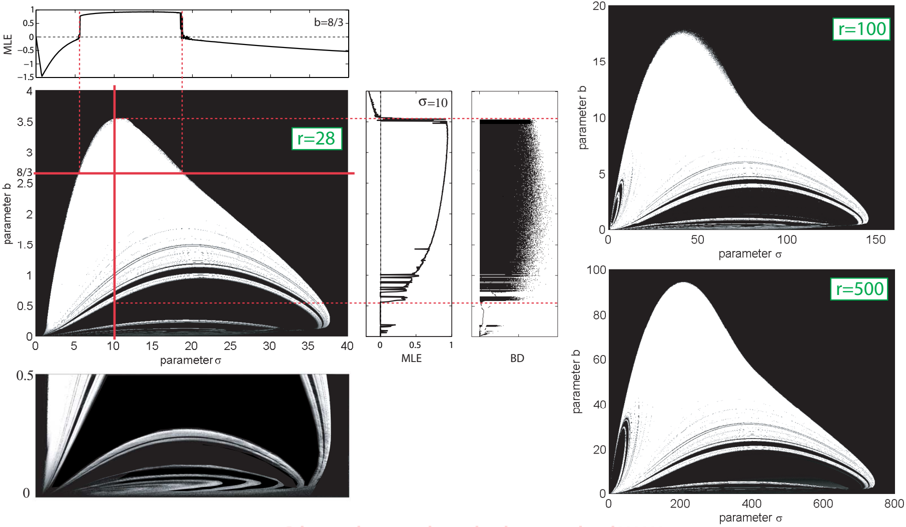
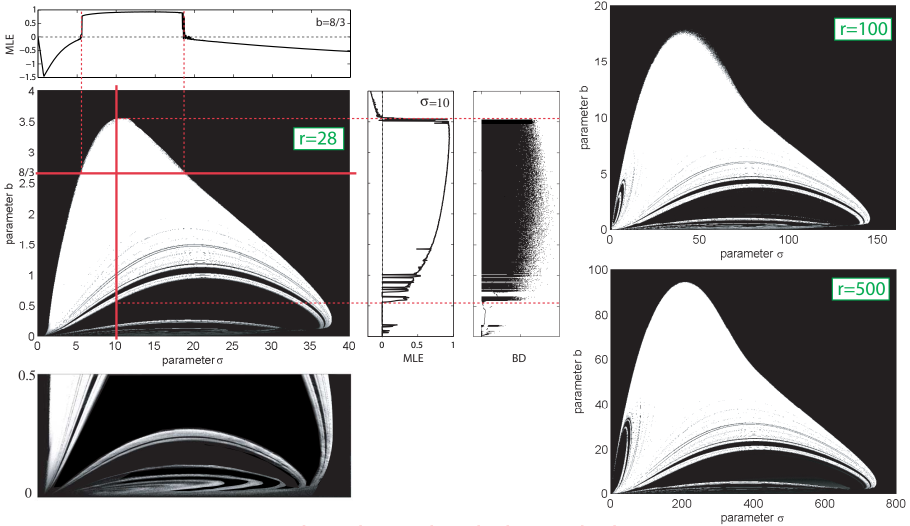
Biparametric analysis: *r* fixed



Chaotic region is bounded!!!!!!

Biparametric analysis: r fixed



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Biparametric analysis: bifurcations

- Software: AUTO and MATCONT
- Period doubling, fold and Andronov-Hopf bifurcations (analytical)

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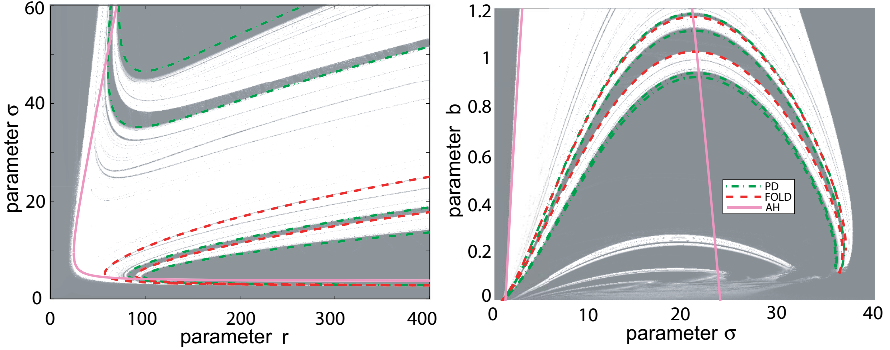
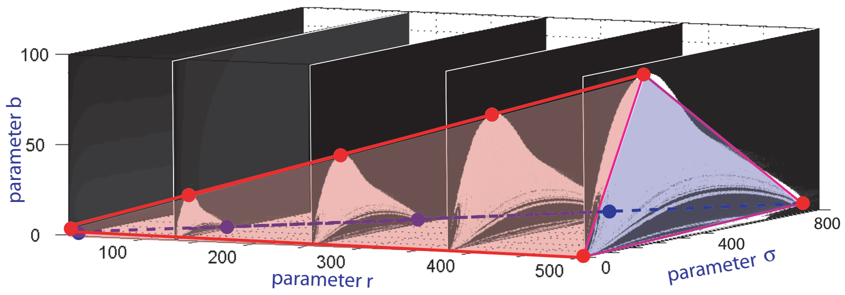
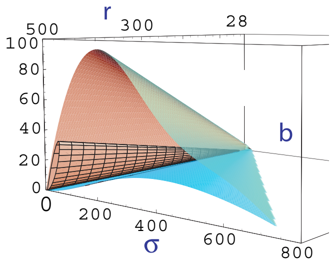
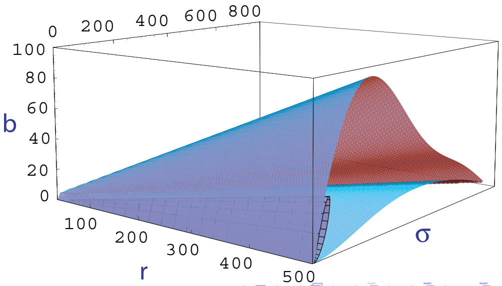


Three-parametric analysis: simplified models

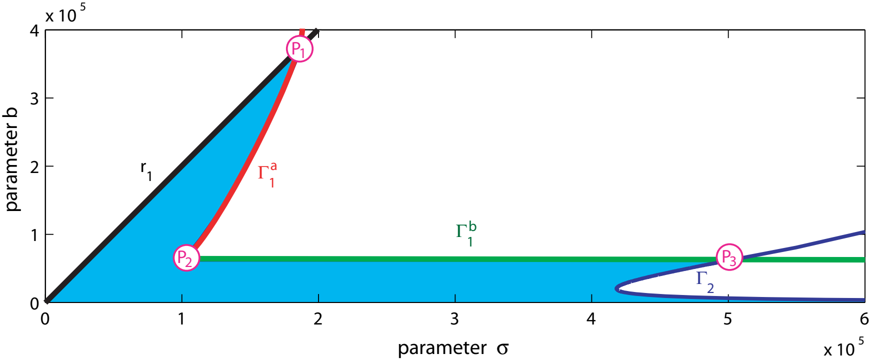






Theorem

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 σ too. To be precise, outside a bounded region every positive semiorbit of the Lorenz system converges to an equilibrium.



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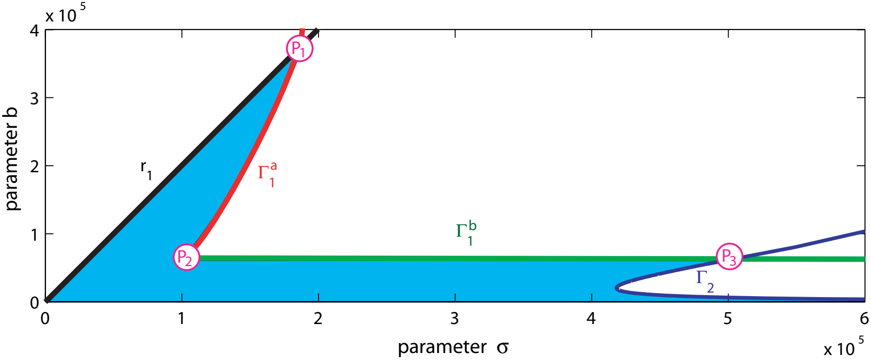

Conjecture

The boundary of the chaotic region in the (σ, b) plane grows linearly with r.

Thank you for your attention :-)