Efficient numerical implementation of integrability criteria based on high order variational equations

Regina Martínez[1] & Carles Simó[2]

(1) Dept. Matemàtiques, UAB

(2) Dept. Matemàtica Aplicada i Anàlisi, UB

reginamb@mat.uab.cat, carles@maia.ub.es

Workshop on
Stability and Instability in Mechanical Systems:
Applications and Numerical Tools

Institut de Matemàtiques

Universitat de Barcelona 0812051230

The problem

To study the integrability of a Hamiltonian $H(q,p)$ real analytic on some domain Ω of $\mathbb{R}^{2n}$. We consider the extension to a complex domain $\hat{\Omega}$ of $\mathbb{C}^{2n}$.

If $x = \{q,p\} \in \mathbb{C}^{2n}$ we consider solutions $x(t)$ with $t \in \hat{D} \subset \mathbb{C}$. The image of $\hat{D}$ by x is a **Riemann surface** Γ. We shall **complete** Γ adding fixed points, singularities and points at infinity to obtain $\bar{\Gamma}$.

We shall consider integrability in the **Liouville-Arnol'd** sense:

There exist n first integrals $f_1, f_2, \ldots, f_n$ independent almost everywhere and in involution. Usually it is taken $f_1 = H$. In general the functions $f_1, f_2, \ldots, f_n$ will be considered **meromorphic in a neighbourhood of a given solution** $x(t)$.

Typically Hamiltonian systems are **non-integrable**.

The problem is **how to detect/prove** the **non-integrability**.

Theoretical results: using first order variational equations

We present results based of **differential Galois theory** because:

1) They do not require to be in the **perturbative setting** $H = H_0 + \varepsilon H_1$,

2) They can be extended to **variational equations of higher order**.

Consider the **ODE** $\dot{x} = f(x(t)), x(t_0) = x_0$ a **regular** point of f, $x \in \mathbb{C}^m$.
Let $x(t)$ be a **solution**.
The **first VE** along $x(t)$ is $\frac{d}{dt}A = Df(x(t))A,\ A(t_0) = Id$.
Consider **closed paths**, γ, on Γ with base point x_0. One can associate to each γ the corresponding monodromy matrix M_1^γ. The set of all these matrices form the **monodromy group** M_1.

In general let

$$\frac{d}{dt}A = B(t)A(t),$$

with the entries of B in a suitable **field of functions** K, the **meromorphic functions on** $\bar{\Gamma}$, and let $\xi_{i,j}$ be the **elements of a fundamental matrix**. Consider the **extension** $L = K(\xi_{1,1}, \xi_{2,1}, ..., \xi_{m,m})$.
$G =$Gal$(L \mid K)$ denotes the **Galois group** of the extension.

The **closure** of the monodromy group is the Galois group.

Theorem 1 (**Morales–Ramis** *Meth. & Appl. of Analysis* **8**, 2001) Under the assumptions above if a Hamiltonian is integrable in a neighbourhood of Γ then the **identity component** G^0 of the Galois group of the first order VE along Γ is **commutative**.

G^0 commutative $\Longrightarrow$ nothing against integrability.

This can happen, typically, for families of Hamiltonian systems depending on parameters, for some exceptional sets of parameters.

This suggests to try to detect **non-integrability** using **higher order variational equations**, methods introduced recently.

Recalling some concepts

Galois group $G = \mathrm{Gal}(L \mid K)$: automorphisms of L which leave K invariant.

It is an **algebraic group**: The elements satisfy some algebraic conditions (polynomials in an ideal in $\mathbb{C}[X_1, ..., X_m]$) and the group operation and passing to the inverse are algebraic.

Whenever we refer to some topological concept (closure, component,...) one should understand that the **Zariski's topology** is used.
The closed sets are the zeros of an ideal. Note that any two open sets are not disjoint. In particular it is not Hausdorff.

Using higher order variational equations

Let $\varphi(t, x_0)$ be the solution of $\dot{x} = f(x(t))$ with $\varphi(0, x_0) = x_0$.

We consider as **fundamental solutions of the k-th order VE, VE$_k$** based on x_0, the string

$$(\varphi^{(1)}(t), \varphi^{(2)}(t), \ldots, \varphi^{(k)}(t))$$

such that

$$\varphi(t, y_0) = \varphi(t, x_0) + \varphi^{(1)}(t)(y_0 - x_0) + \ldots + \varphi^{(k)}(t)(y_0 - x_0)^k + \ldots,$$

i.e., **the coefficients of the k-jet**.

$\varphi^{(k)}(t)$ satisfy **linear non-homogeneous ODE**.

$\frac{d}{dt}\varphi^{(k)}$, $k > 1$ depends on $\varphi^{(j)}$ for $j < k$ in a **nonlinear way**. It can be made linear by **adding additional variables**.

Then one can introduce the **k-th order Galois group G_k**. Loosely we can talk about the **k-th order monodromy M_k^γ** along a path γ.

The **composition** of elements in M_k^γ as a group is equivalent to the **composition of jets**.

Theorem 2 (**Morales–Ramis–S** *Ann. Scient. Éc. Norm. Sup.* 4^e série **40**, 2007)
Under the assumptions above if a Hamiltonian is integrable in a neighbourhood of Γ then for any $k \geq 1$ **the identity component** $(G_k)^0$ **of** G_k **is commutative**.

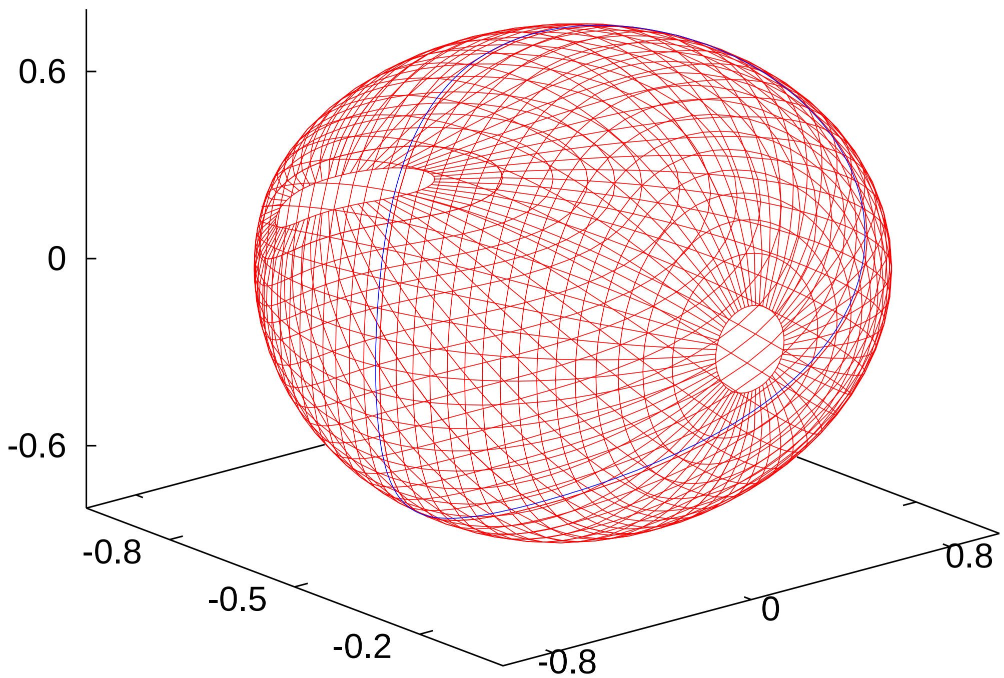
This result gives rise to **non-integrability criteria to all orders**. Note that these criteria can depend strongly on the reference solution $x(t)$ and on the paths taken on it.

A degenerate Hénon-Heiles problem

Hénon-Heiles family (HHF) (classical $b = -1$):

$$H = \frac{1}{2}(x_3^2 + x_4^2 + x_1^2 + x_2^2) + \frac{1}{3}x_1^3 + bx_1x_2^2,$$

non-integrable for all b except **four values**. For **3 of them** integrability is proved. Remaining case: $b = 1/2$, degenerate Hénon-Heiles **DHH**. Fixed points $P_{ee} = (0, 0, 0, 0)$, $P_{hp} = (-1, 0, 0, 0)$.



The global W^c_{hp} manifold. Coincides with a family of periodic orbits.

Separatrix Γ_0 on the invariant plane $\{x_2 = x_4 = 0\}$ and $H = h_0 = 1/6$:

$$x_1(t) = \frac{3/2}{\cosh^2(t/2)} - 1, \quad x_3(t) = \frac{-(3/2)\sinh(t/2)}{\cosh^3(t/2)}, \quad \textbf{singularity } t_* = \pi \mathrm{i}\,.$$

Double-periodic solutions for $h < h_0$: ψ_1, ψ_2 paths along real, imaginary periods. Then

$$[M_k^{\psi_1}, M_k^{\psi_2}] = M_k^{\psi_2^{-1}} \circ M_k^{\psi_1^{-1}} \circ M_k^{\psi_2} \circ M_k^{\psi_1}$$

should be trivial. Path **can be deformed** to loop γ around t_*.

Reduces to **local checks**: M_2^γ trivial, but some components of $\varphi^{(3)}$ are **different from zero**. E.g. $x_{2;2,2,2} = \frac{72}{5} 2\pi \mathrm{i}\,.$

In general we can have solutions with **several singularities** and we can have also **new singularities** in the coeficients of the variational equations. If $(G_1)^0$ or $(M_1)^0$ is commutative we have to go to **higher order variational equations**.

A monodromy matrix M is in $(G_1)^0$ if, for instance, $M = \begin{pmatrix} 1 & a \\ 0 & 1 \end{pmatrix}$.

Solutions of VE_k, $k > 1$ are obtained from solutions of VE_1 by **quadrature**.

Problems in checking the necessary conditions

To apply **Theorem 2** to concrete systems several **difficulties** are found:

- To apply these methods one needs to use an **explicitly** known solution $x(t)$.
- They require the choice of a **suitable path** for the complex time.
- In general it is **not possible to integrate analytically first and higher order variational equations** in a simple and efficient way.

The need of higher order VE to prove **non-integrability** can be independent of the existence of **large chaotic regions** in numerical simulations. **Simple enough** solutions can be more **degenerate** than a generic one.

Ergo $\Longrightarrow$ **numerical check of the necessary conditions for integrability** along arbitrary paths γ of $t \in \mathbb{C}$.

A method with a wide range of applications, based on **Taylor expansions both in time and in nearby initial conditions**, is presented. The integration of **arbitrary higher order VE along arbitrary paths** is easily automatized.

The Taylor method for the numerical integration of ODE

Problem: to integrate $\dot{x} = f(t,x)$, $x(t_0) = x_0$,.
f analytic in a neighbourhood of $(t_0, x_0) \in \Omega \subset \mathbb{R} \times \mathbb{R}^n$ or $\Omega \subset \mathbb{C} \times \mathbb{C}^n$.

From $x(t_0+h) = \sum_{j\geq 0} c_j h^j$ and $f(t_0+h, x(t_0+h)) = \sum_{j\geq 0} d_j h^j$ it follows $c_j = d_{j-1}/j$. It remains **to compute the** d_j.

This is done in a **recurrent way**. Assume to evaluate f can be split in **simple expressions**:

$$\begin{aligned}
e_1 &= g_1(t,x), \\
e_2 &= g_2(t,x,e_1), \\
&\vdots \\
e_j &= g_j(t,x,e_1,\ldots,e_{j-1}), \\
&\vdots \\
e_m &= g_m(t,x,e_1,\ldots,e_{m-1}), \\
f_1(t,x) &= e_{k_1}, \\
&\vdots \\
f_n(t,x) &= e_{k_n},
\end{aligned}$$

where each of the e_j contains a sum of arguments, a product or quotient of two arguments or an **elementary function** (like $\sin, \cos, \log, \exp, \sqrt{}, \ldots$) of a **single argument**.

Inserting $c_0 = x_0$ in the e_j we obtain d_0 and then c_1. Putting $x(t_0) = c_0 + c_1 h$ all the e_i can be obtained to order 1 in h. Then we have d_1 and hence c_2. **Iterate to the desired order**. All the g_j can be seen as **operations with (truncated) power series**.

Examples: If $a(h) = \sum_{k\geq 0} a_k h^k, \quad b(h) = \sum_{k\geq 0} b_k h^k$

$$c = a \times b : \quad c_n = \sum_{k=0}^{n} a_k b_{n-k}$$

$$c = a^\alpha,\ \alpha \in \mathbb{R},\ a_0 \neq 0, \quad c_0 = a_0^\alpha,$$
$$c_n = -\frac{1}{n a_0} \sum_{k=0}^{n-1} c_k a_{n-k} [k - \alpha(n-k)],\ n > 0$$

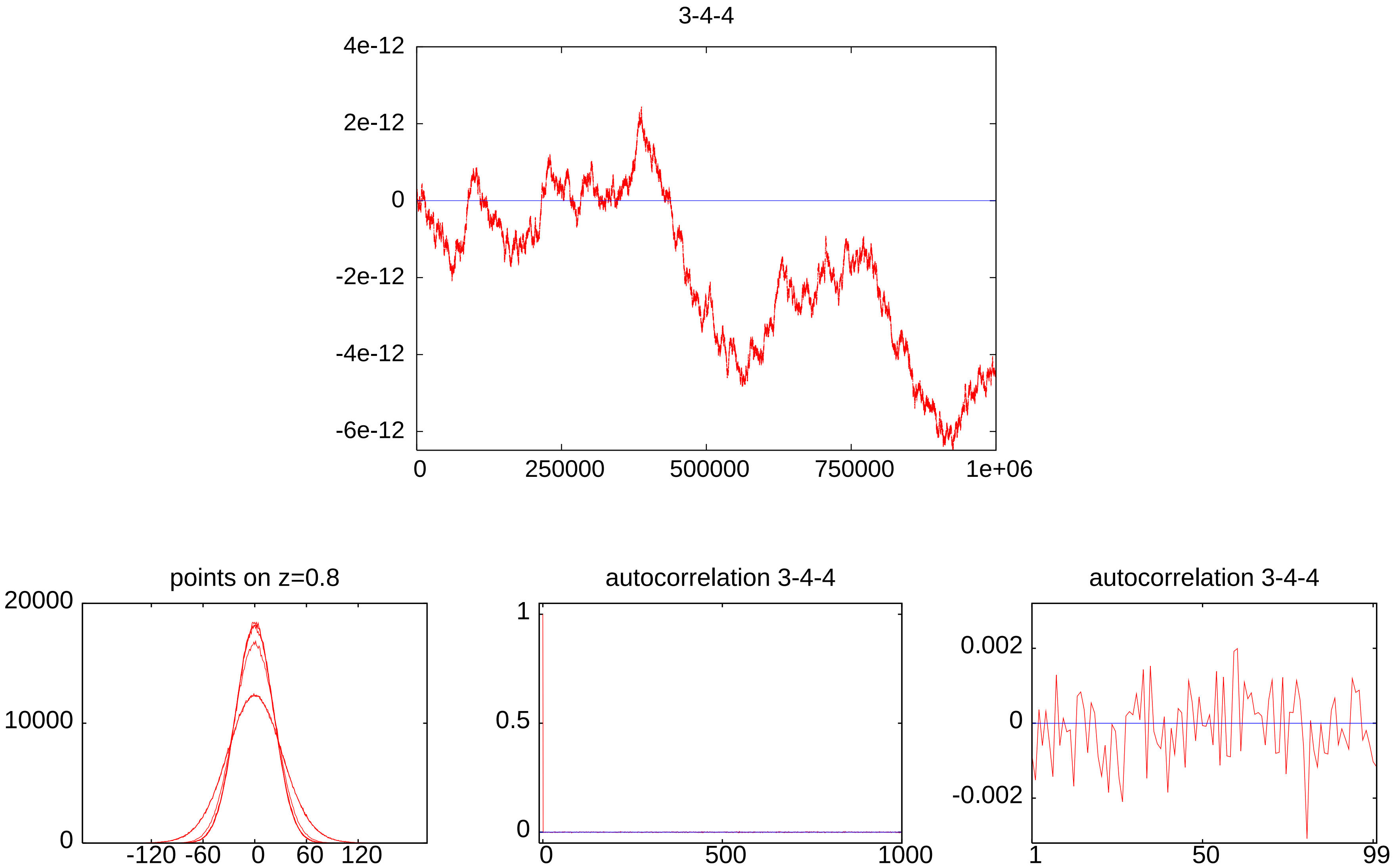
$$c = \exp(a), \quad c_0 = \exp(a_0), \quad c_n = \frac{1}{n} \sum_{k=0}^{n-1} c_k a_{n-k} (n-k),\ n > 0$$

Suitable for analytic (or regular enough) f, non-stiff.

Some interesting properties

- Under simple conditions **optimal stepsize** (concerning efficiency for fixed truncation error) ≈ independent of the number of digits. $h_{\rm opt}$ close to $\rho(t)/\exp(2)$, where $\rho(t)$ = local radius of convergece around t.
- **optimal order** $N_{\rm opt}$ ≈ linear in the number of digits.
- The **computational cost** to integrate from t_0 to t_f (measured in number of elementary operations) ≈ quadratic in the number of digits.
- It is elementary to produce **dense output**.
- Very simple application to obtain **Poincaré sections**.
- Domain of **absolute stability** ≈ $|z| < N/e$, $\mathrm{Re}(z) < 0$.
- Easy to reduce errors to the propagation of **round off**.

See paper and software by À. Jorba, M. Zou, *Experimental Mathematics* **14** (2005) 99–117.
Also: C. Simó, Taylor method for the integration of ODE, Lecture notes, available at `http://www.maia.ub.es/dsg/2007/`.



Example of use of Taylor method: RTBP Sun-Jupiter-Trojan with initial $z = 0.8$. Worst case. Integration time$=10^9$ Jupiter revolutions $\approx$ **2.6 times the age of the Solar System**.

Jet transport

Problem: Given initial conditions $x_0 + \xi$ to obtain $\varphi(t; t_0, x_0 + \xi) = \varphi(t; t_0, x_0) + Q(t; t_0, x_0, \xi) = P(t; t_0, x_0, \xi) = \sum_m a_m(t)\xi^m$, where P is a **polynomial truncated at the desired order**.

Example: in $\mathbb{R}^4$ integrate to degree 3 in ξ. Using **variational equations** requires $4+16+64+256 = 320$ equations, which reduce to 140 by symmetry.

A simpler method: Integrate using **any method (e.g.Taylor)** but replacing **operations with numbers** by **operations with polynomials truncated at the desired order**.

Strongly related to the **Taylor models** largely used by M. Berz, K. Makino and collaborators, see, e.g. `http://bt.pa.msu.edu/berz`.

If $P(\xi), Q(\xi)$ are polynomials up to (total) order k the recurrences mentioned in Taylor method can be used to obtain, to order k, the polynomials corresponding to $P \times Q$, P^α, $\exp(P)$, ...

Remark: in the selection of the **optimal step size** one has to take into account **all the a_m coefficients**.

Some systems requiring order k variational equations

As an extension of DHH consider, for $m \geq 2$, the **generalised degenerate HH** problem, GDHH, with Hamiltonian

$$H = \frac{1}{2}(x_3^2 + x_4^2) + \frac{1}{2}x_1^2 + \frac{1}{3}x_1^3 + (1 + x_1)\frac{1}{n!}x_2^n.$$

For $n = 2$ gives DHH. Consider now $n \geq 3$. As proved in Martínez-S (2008a) these systems require to go to **order $n - 1$** to detect **non-integrability** close to a separatrix like in the DHH case.

Singularities located at $t = (2k + 1)\pi \mathrm{i}$; a suitable path is OABCDO, where: O$= (0, 0)$, A$= (2, 0)$, B$= (2, 6)$, C$= (-2, 6)$, D$= (-2, 0)$. Initial point: close to symmetric point on the separatrix, i.e., $(r, 0, 0, 0)$, $r \approx 1/2$.

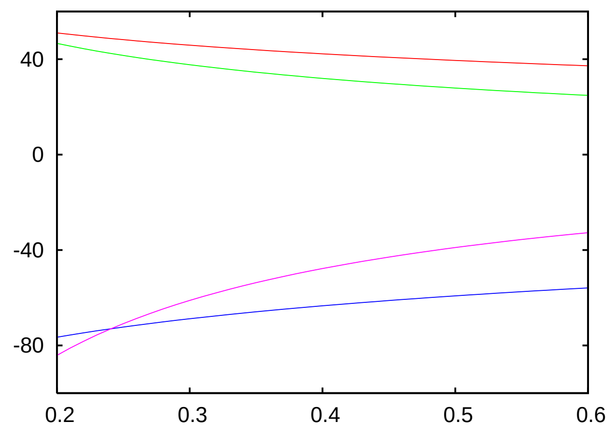
Notation: $a_{i;k_1,\ldots,k_n}(t)$ = coefficient of $\xi_1^{k_1} \ldots \xi_n^{k_n}$ in the i-th component of $P(t; t_0, x_0, \xi)$. Simply $a_{i;k_1,\ldots,k_n}$ at the end of path γ.

Results

If $1 < |k| < n - 1$ only round off errors (e.g., $< 10^{-8}$ if $n < 12$).
If $n = 7$ only non-zero for $i \in \{2, 4\}$, $k_1 = k_3 = 0$, $k_2 + k_4 = 6$.

$a_{2;0600}$	-0.52359878E-01 i		
$a_{2;0501}$	0.19739209E+01	$a_{4;0501}$	0.31415927E+00 i
$a_{2;0402}$	0.23254708E+02 i	$a_{4;0402}$	-0.49348022E+01
$a_{2;0303}$	-0.12987879E+03	$a_{4;0303}$	-0.31006277E+02 i
$a_{2;0204}$	-0.38252461E+03 i	$a_{4;0204}$	0.97409091E+02
$a_{2;0105}$	0.57683352E+03	$a_{4;0105}$	0.15300984E+03 i
$a_{2;0006}$	0.35236754E+03 i	$a_{4;0006}$	-0.96138919E+02

which **coincide with theoretical values** to all digits displayed.



Values of four non-zero coefficients of the jet at order 4 after a loop around the singularity for the GDHH problem with $n = 5$, as a function of the initial point $x_0 = (r, 0, 0, 0)$. The other two non-zero coefficients do not change with r.
Other systems with $x_1^2/2 + x_1^3/3$ replaced by **higher order polynomials** (up to degree 12) give similar results. Separatrix **not available analytically**.

A nonlinear spring-pendulum problem

The Hamiltonian

$$H = \frac{1}{2}\left(x_3^2 + \frac{x_4^2}{x_1^2}\right) - x_1 \cos(x_2) + \frac{k}{2}(x_1 - 1)^2 - \frac{a}{3}(x_1 - 1)^3, \; k > 0$$

Known results (Maciejewski-Przybylska-Weil, *J. Phys. A* **37**, 2004):

If $k + a \neq 0,\ k > 0$ the system is **non-integrable**.

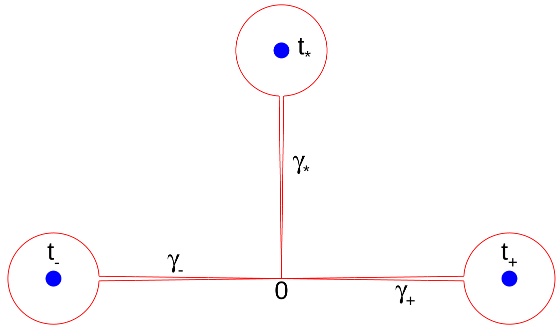
A simple solution for $a = -k$

$$x_1(t) = \rho + \frac{\alpha}{\cosh^2(\beta t)}, \quad x_3(t) = \dot{x}_1(t) \quad x_2 = x_4 = 0,$$

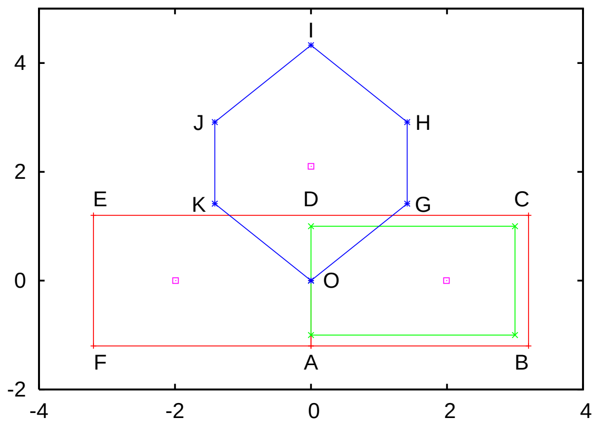
with ρ, α, β **depending on** k. It has a **singularity** at $t_* = \frac{\pi \mathrm{i}}{2\beta}$.
MPW checked that for $a = -k$ **no obstruction** appears up to order 7.

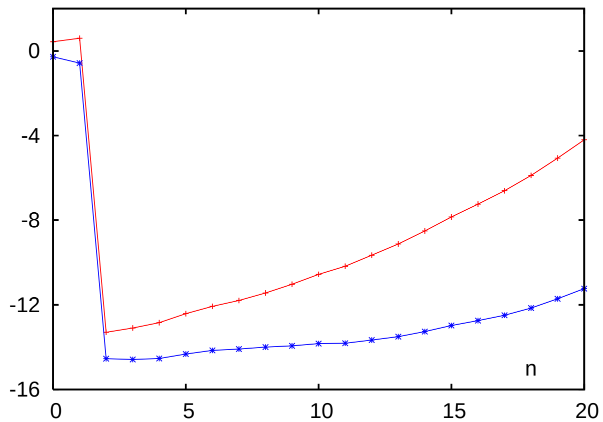
But **other singularities** appear for the VE at $\pm\hat{t}$, where $x_1(\pm\hat{t}) = 0$.

$$\pm\hat{t} = \pm\frac{1}{\beta}\log\left(\sqrt{-\frac{\alpha}{\rho}} + \sqrt{-\frac{\alpha}{\rho} - 1}\right)$$



Path to study of the nonlinear spring pendulum around the three singularities of the variational equations. Equivalent to a **commutator path**.



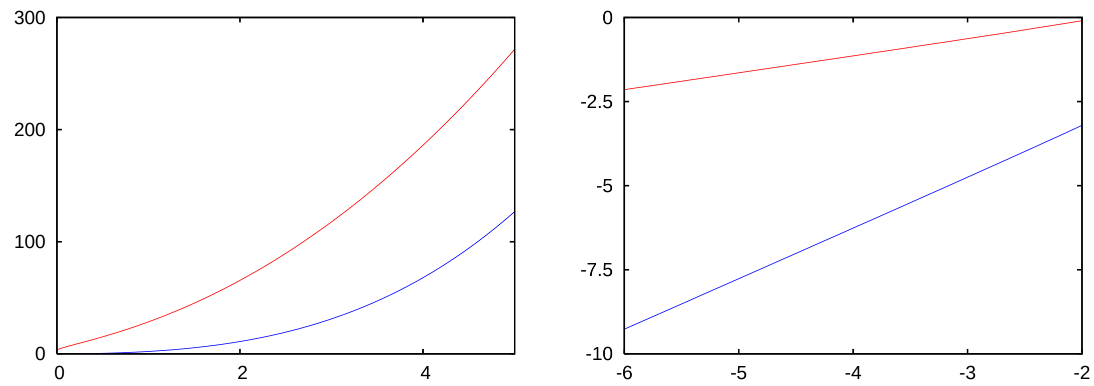


Left: Sample of paths used for the jet transport and location of singularities. γ_+ around t_+ is OABCDO, $\gamma_\pm$ around t_+ and t_- is OABCEFAO, and γ_* around t_* is OGHIJKO. Right: Computed sums of the norms of all terms in the jets at order n (upper curve) and value normalized by the maximum for every order, along γ_*. Vertical variable in $\log_{10}$ scale.

Next step is to check the **jet transport along** $\gamma_\pm$. First we do it along γ_+. The results obtained are of the form

$$T_{\gamma_+}(\xi) = \begin{pmatrix} \xi_1 \\ \xi_2 + a\mathrm{i}\,\xi_2^3 - c\mathrm{i}\,\xi_2^2\xi_4 + 3d\mathrm{i}\,\xi_2\xi_4^2 - e\mathrm{i}\,\xi_4^3 \\ \xi_3 \\ \xi_4 + b\mathrm{i}\,\xi_2^3 - 3a\mathrm{i}\,\xi_2^2\xi_4 + c\mathrm{i}\,\xi_2\xi_4^2 - d\mathrm{i}\,\xi_4^3 \end{pmatrix} + \mathcal{O}(|\xi|^4),$$

with $a, b, c, d, e > 0$. Symplectic character is checked. Similar for γ_-. For $\gamma_\pm$ only $0, 2b, 0, 2d, 0$ subsist. Theoretical results (Martínez-S, 2008a) **agree qualitatively** (no explicit values could be computed theoretically).



Left: Values of $a_{2;0300}$ (upper curve) and $-a_{4;0003}$ (lower curve) as a function of k at the end of $\gamma_\pm$. Right: magnification in $\log_{10}$ scale for $a_{2;0300} - 3$ and $-a_{4;0003}$.

The Swinging Atwood's Machine

A classical mechanical device. If we **include pulleys** the Hamiltonian is

$$H(r,\theta,p_r,p_\theta)=\frac{1}{2}\left[\frac{p_r^2}{M_t}+\frac{(p_\theta+Rp_r)^2}{mr^2}\right]+gr(M-m\cos\theta)+gR(m\sin\theta-M\theta),$$

where $M_t = M + m + 2\frac{I_p}{R^2}$.

Theorem (PPSRMWS, Swinging Atwood's machine: experimental and theoretical studies, preprint 2008):
For every physically consistent value of the parameters, the SAM with pulleys is meromorphically non-integrable.

This can be already detected using Theorem 1.

Without pulleys and normalising constants

$$H = (x_3^2/(1+\mu) + x_4^2 x_1^{-2})/2 + x_1(\mu - \cos(x_2)),$$

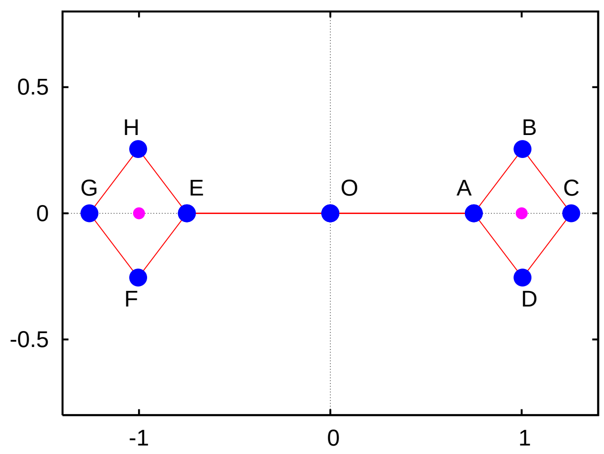
where μ is a mass ratio, $\mu > 1$ in the domain of interest.

Known to be **non-integrable if $\mu \neq \mu_p$** where $\mu_p = 1+\frac{4}{p^2+p-4}$, $p \in \mathbb{N}$, $p>2$ and integrable if $\mu=\mu_2=3$. (Casasayas- Nunes-Tufillaro, *J. Physique* **51**, 1990).

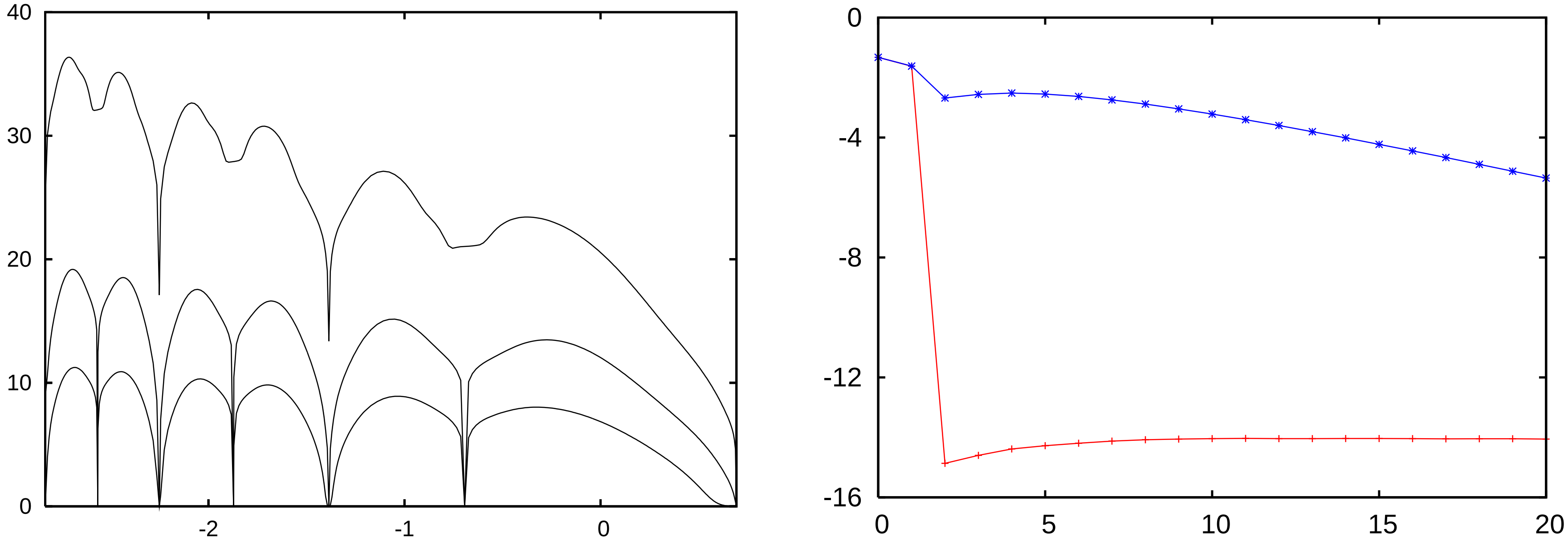
It remains to study the **exceptional cases**, which can not be decided using Theorem 1. **Non-integrability proved** in Martínez-S, 2008b.
A simple solution

$$x_1(t) = \frac{1}{a}\left(1 - t^2\right), \quad x_2(t) = 0, \quad x_3(t) = (1 - \mu_p)t, \quad x_4(t) = 0,$$

where $a = p^2 + p - 2$. Note that $r(t_\pm) = r(\pm 1) = 0$.
Several paths have been taken for the tests. We recall that **the path associated to the commutator** must travel around t_+ and t_- and then again around them reversing orientation: $\gamma_-^{-1} \circ \gamma_+^{-1} \circ \gamma_- \circ \gamma_+$.
Let $g^{(s)} = \sum_{i=1}^{4} \sum_{n \in ^4, |n|=s} |a_{i;n_1,n_2,n_3,n_4}|$ a **norm of the terms of order s** and define a **relative error** $\varepsilon^{(s)} = g^{(s)}(t = t_{\text{final}}) / \max_{t \in \gamma_*} \{g^{(s)}(t)\}$.

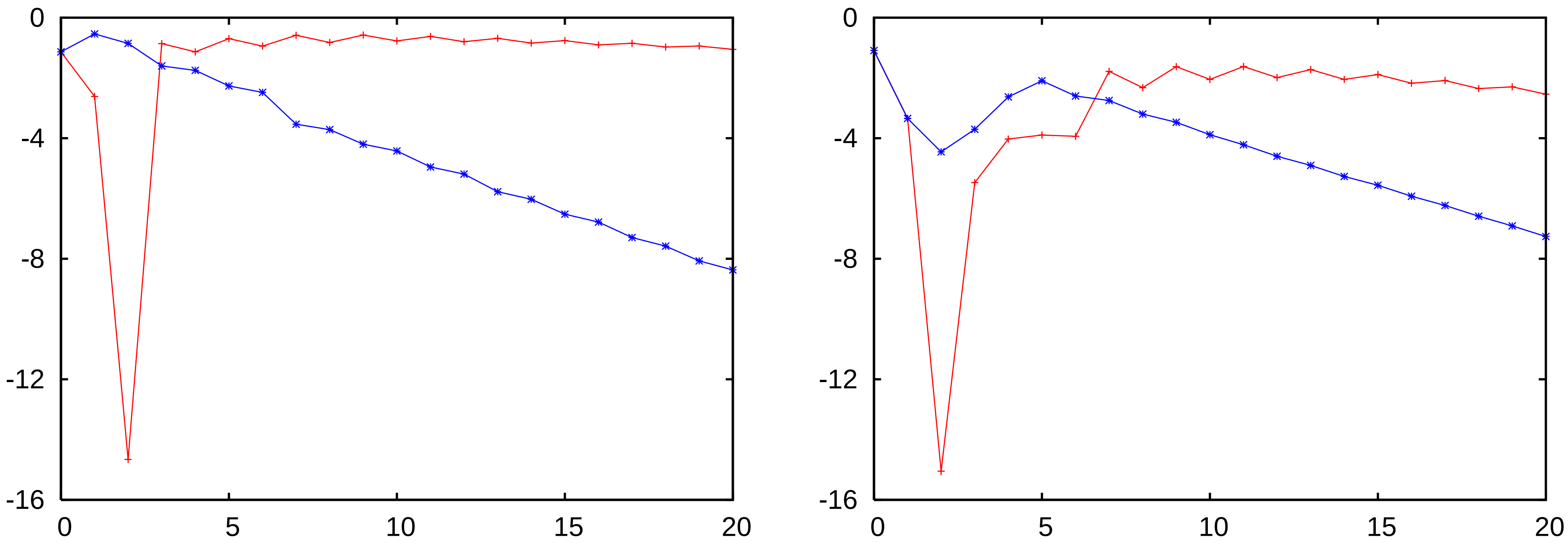


One of the paths, OABCDAOEFGHEOADCBAOEHGFEO, used for tests.

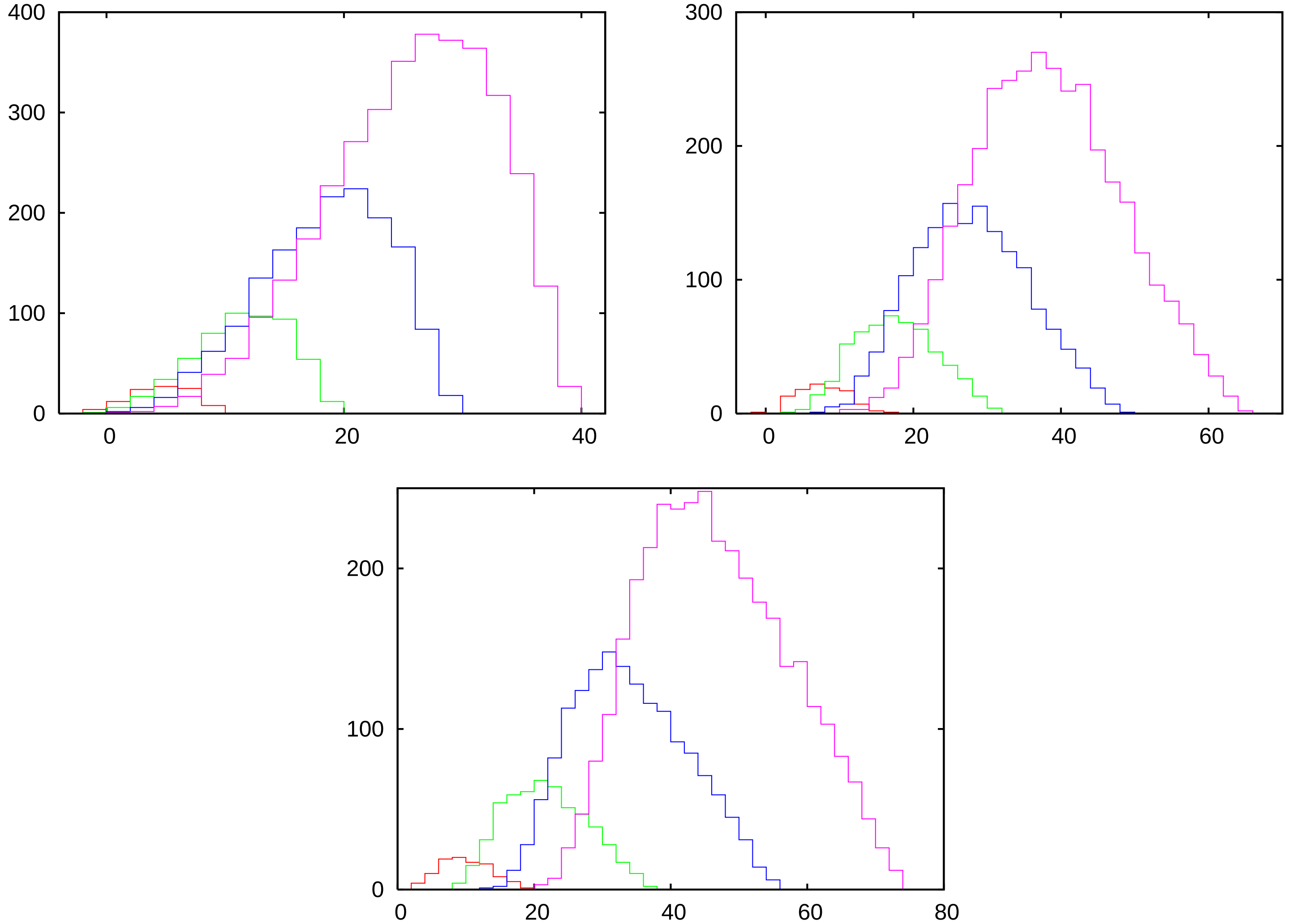


Left: The norms $g^{(s)}$, of the terms of **order 1,2 and 3** for SAM as a function of μ. The lower (resp. upper) curve corresponds to $s = 1$ (resp. $s = 3$). For $s = 1$ we show the change with respect to the identity matrix. In the horizontal axis we display $\log(\mu - 1)$ while in the vertical one $\operatorname{arcsinh}(g^{(s)})$ is shown.

Right: For $p = 2$ we consider the values of $g^{(s)}$ **at the end of** Γ (lower curve) and of γ_+ (upper curve) divided by the maximal value of $g^{(s)}$ along the full path, as a function of s. For both curves in the vertical axis the $\log_{10}$ scale has been used.



Plots similar to the previous one for $p = 3$ (left) and $p = 4$ (right). Now, in contrast with the case $p = 2$, the lower upper (lower curve), at least for large s, corresponds to the $\log_{10}$ of the quotient of $g^{(s)}$ at the end of γ_+ (**at the end of** Γ) by the maximal value of $g^{(s)}$ along the full path. Note that now the final value (except for the known cases $s = 1, 2$) is only one or two orders of magnitude smaller than the maximal value.



Histograms of the **number of elements** $a_{i;n_1,n_2,n_3,n_4}$, $n \in \mathbb{N}^4, |n| = s$ such that the $\log_{10}$ of its **maximum value along** Γ is in a **given range**. On the top left (resp. right, bottom) appear the results for $p = 2$ (resp. $p = 3$, $p = 4$). In each plot the values for $s = 5, 10, 15, 20$ are shown.

Final considerations

We have used the **check of Theorem 2** as an application of **jet transport**.

a) One can convert the computation into a **rigorous proof, CAP**, by using **interval arithmetic** and estimates of **remainder** in Taylor using Cauchy bounds.

b) A **difficulty** shows up to extend this to **unbounded ranges** of parameters. **Analytical proofs** can not be avoided in general.

c) Jet transport is **even efficient!**. On the plot for a range of μ in the SAM, the **average computing time** per value of μ is **24 ms**. In that time one can compute **only one hundred of Poincaré iterates!**

Some further applications of jet transport:

1) Transport of a **box of initial data** under the flow, assuming that the image is not too large. Otherwise, add the use of **subdivision** methods.

2) Transport of **probability distributions** under the same assumptions.

3) Computation of **high order approximations of return maps** associated to any type of connection.

4) Computation of **normal forms** around arbitrary orbits. Application to obtain **local expansions of $W^{u,s,c}$**, to study **higher order codimension bifurcations**, check assumptions for validity of **KAM theorems**, etc.