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Backward error analysis of numerical methods for ODEs and Lie–Hori perturbation theory

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Abstract

Backward error analysis of numerical methods for ordinary differential equations has proved to be in recent times a valuable tool to study the geometric properties of numerical integrators [3]. In this approach the numerical solution is the exact solution of a new differential equation which is a perturbation of the original equation in which the step size appears as small parameter. Clearly such an approach is closely related with perturbation theories that have been widely used in Celestial Mechanics to approximate the solution of some dynamical systems. The aim of this paper is to give a brief view of backward error analysis and to show its connection with Lie–Hori perturbation theory.

Key words and expressions: Numerical integration of ODEs, backward error analysis, modified equations, Lie–Hori perturbation theory.

MSC: 65L05, 65M20.

1 Introduction

In the numerical solution of initial value problems for ODEs

$$\frac{d}{dt}y(t) = f(y(t)), \quad t \geq 0, \quad y(0) = y_0 \in \mathbf{R}^m \tag{1}$$

by means of one step methods with a fixed step size one gets a discrete solution $(y_j)_{j\geq 0}$ that approximates the exact solution $y(t)$ of (1) at the uniformly spaced grid points $t_j = jh, j = 0, 1, \ldots$. The approximations $y_{j+1} = \phi_h(y_j), j = 0, 1, \ldots$ are computed recursively by a map $\phi_h = \phi_{h,f}$ that depends on the vector field f of (1) , the numerical method and the step size h.

A standard measure to test the quality of a given method $\phi_{h,f}$ is the so called local error defined at each y_n by $\|\Phi_{h,f}(y_n) - \phi_{h,f}(y_n)\|$ where $\Phi_{t,f}$ is the time–t flow map of (1), i.e. $\Phi_{t,f}(y_n)$ is the solution of the differential equation of (1) starting from the point y_n at $t = 0$. A method $\phi_{h,f}$ has order p if its local error behaves as $\mathcal{O}(h^{p+1})$ when $h \to 0^+$ for all f sufficiently smooth. Further this fact implies that the global error, i.e. the error after N steps with Nh moderately sized, behaves as $\mathcal{O}(h^p)$ when $h \to 0^+$. This forward error analysis has been the basis to construct most of the standard numerical methods in use for solving ODEs.

An alternative approach to study the error behaviour of a method $\phi_{h,f}$ is to consider the numerical solution (y_n) as the exact flow of another vector field $\widetilde{f}(y;h)$ depending on the constant step size h

$$\frac{d\widetilde{y}(t;h)}{dt} = \widetilde{f}(\widetilde{y}(t;h);h), \quad t \geq 0 \qquad \widetilde{y}(0;h) = y_0, \tag{2}$$

at the grid points $t_j = jh$, so that $\Phi_{t_j,\widetilde{f}}(y_0) = \widetilde{y}(t_j;h) = y_j$, for all $j = 0, 1, \ldots$. Provided that such an equation (2) exist, it is usually called the modified equation of (1) associated to the method $\phi_{h,f}$. Hence the comparison of the flows of the original equation (1) and the modified equation (2) allows us to assess the quality of a method. In this approach called Backward Error Analysis (BEA) the numerical solution generated by a method with step size h is the exact solution of a differential system (2) that can be considered as a perturbation of the original system (1).

It must be noticed that, as remarked by several authors [3, 7, 1] BEA, in conjunction with some perturbation results for differential equations, permits to derive not only error bounds for the numerical solution but also other results on the preservation of qualitative properties of the original differential system and the long term behaviour of numerical methods. On the other hand (2) may be viewed as a perturbed system of (1) with the step size as a small parameter and it is well known that there is a long experience with perturbation methods in the field of Celestial Mechanics [2, 5, 4, 6] and in this context the aim of this paper connecting the two fields is two fold: First of all to show that the modified equations (2) of (1) associated to the method $\phi_{h,f}$ can be considered as a Lie–Hori type generator [5] of the near identity map $\phi_{h,f}$ and therefore some algorithms used to derive the Lie–Hori transformations can be applied to BEA. Secondly, it is expected that linking BEA and perturbation theories of Celestial Mechanics will allow researchers of both fields to exchange techniques and tools useful to their problems of interest.

The paper is organized as follows: In section 2 some well known remarks on the modified equations are briefly collected. In section 3 the relevant algorithms of the Lie-Hori perturbation theory for general (non Hamiltonian) differential equations are presented making clear its connection with BEA. Finally in section 4 some numerical examples are given to illustrate the applicability of Lie–Hori techniques to some problems.

2 The Modified Equations

As remarked before it is not evident that given an IVP (1) with f sufficiently smooth and a numerical method $\phi_{h,f}$ there exists a function $\widetilde{f}(y;h)$ for all $h \in [0,h_0], h_0 > 0$ such that the solution $\widetilde{y}(t;h)$ of (2) satisfies $\widetilde{y}(t_n;h) = y_n$ for all $n \geq 0$. However if (1) is a linear system

$$y' = f(y) = S\, y, \tag{3}$$

with a constant matrix S and ϕ_h is the map generated by a Runge–Kutta method ($A \in \mathbf{R}^{s\times s}, b \in \mathbf{R}^s$) with stability function $R(z) = 1+z\, b^T(I-zA)^{-1}e$ with $e = (1,\ldots,1)^T \in \mathbf{R}^s$, then ϕ_h is the linear map $\phi_h(y_0) = R(hS)\, y_0$, and for $t = nh$, we have

$$y_n = \phi_h(y_{n-1}) = [R(hS)]^n\ y_0 = [R(hS)]^{(t/h)}\ y_0 = \exp\left[t\ h^{-1}\ \log(R(hS)\right]\ y_0,$$

and therefore a continuous function $\widetilde{y}(t;h)$ such that $\widetilde{y}(nh;h) = y_n$ can be taken as the solution of the linear system

$$\widetilde{y}' = [(1/h)\ \log(R(hS))]\ \widetilde{y}, \qquad \widetilde{y}(0) = y_0. \tag{4}$$

Now, since $R(z)$ is a rational approximation to the exponential, there exist some $h_0 > 0$ such that the h–power series expansion of $(1/h)\ \log(R(hS))$ has a positive radius of convergence. Thus for a linear system (3) and a Runge–Kutta method there exists a modified equation (4) with the vector field $\widetilde{f}(y;h)$ given as a power series of h with a positive radius of convergence.

For non linear functions it must be noticed that even for an analytic function $f(y)$ in a neighbourhood of the initial point y_0 and very simple methods the modified equation is an asymptotic expansion that does not converge. To illustrate this fact consider the case of a quadrature

$$y'(t) = f(t), \qquad y(0) = 0, \tag{5}$$

with an arbitrary analytic function $f(t)$. Note that although the equation is non autonomous it can be written as a two dimensional autonomous system with the state vector $(t,y)^T$.

Taking as numerical method the trapezoidal rule $y_{n+1} = y_n + (h/2)[f(y_n) + f(y_{n+1})]$ we have $y((n+1)h) = y(nh) + (h/2)[f(t_n) + f(t_{n+1})]$ whose ϕ_h–map is given by

$$\phi_h(t,y) = y + \frac{h}{2}\left[f(t) + f(t+h)\right].$$

Here it can be seen that the modified equation of (5) is a quadrature that has the form

$$\widetilde{y}' = f(t) + \frac{h^2}{2!}B_2 f''(t) + \frac{h^3}{3!}B_3 f'''(t) + \ldots \tag{6}$$

where B_i are the Bernoulli numbers that behave as

$$B_k \sim \frac{\text{Const.}}{(2\pi)^k}\, k! \qquad (k \to \infty),$$

and for an analytic function f with poles we have

$$\frac{f^{(k)}(t)}{k!} \sim \frac{\text{Const.}}{R^k},$$

then the series in the right hand side of (6) diverges for all $h > 0$.

Leaving aside all convergence matters, it has been usual to assume that the discrete flow map $\phi_{h,f}$ defined by a one step method (typically a Runge–Kutta method) for a step size h and a vector field f, possess a Taylor series expansion in powers of h with the form

$$\phi_h(y) = y + \sum_{j\geq 1} h^j\ \varphi_j(y) \tag{7}$$

and the vector field of the modified equation possess a formal series expansion

$$\widetilde{f}(y;h) = W_1(y) + hW_2(y) + h^2 W_3(y) + \dots \tag{8}$$

with $W_1(y) = f(y)$. Now since (2) is an autonomous system $\widetilde{y}(t_j;h) = y_j = \phi_h^j(y_0)$ holds for all $j = 1, 2, \dots$ if and only if it holds for $j = 1$, i.e. $\widetilde{y}(h;h) = \phi_h(y_0)$ and comparing the Taylor series expansion of the solution of (2), where $\widetilde{f}$ given by (8), with (7) we can get successively the functions W_j. This has been the approach followed by Hairer, Lubich and Wanner in ([3], p. 288).

Another equivalent approach due to Reich [7] proposes to compute recursively the successive modified vector fields

$$\widetilde{f}_i(y;h) = \sum_{j=1}^{i} h^{j-1} W_j(y), \qquad i \geq 1$$

by the recursion $\widetilde{f}_1 = W_1 = f$, and

$$\widetilde{f}_{i+1} = \widetilde{f}_i + h^i W_{i+1}, \quad W_{i+1}(x) = \lim_{h\to 0} \frac{\phi_h(x) - \Phi_{h,\widetilde{f}_i}(x)}{h^{i+1}},$$

where $\Phi_{t,\widetilde{f}_i}$ is the flow–t map of the modified equation with field $\widetilde{f}_i$. This recursion, although it is not practical for the explicit computation of $\widetilde{f}_i$, turns out to be very convenient to study geometric properties of BEA and the long term behaviour of numerical methods.

In spite of the lack of convergence of the vector field (8) of the modified equation, in many cases taking a few terms of this asymptotic expansion the flow defined by this vector field provides an excellent approximation of ϕ_h. A deep result on this line was proved by Benettin and Giorgilli (1994) [1]. Here we present a slightly modified version due to Reich [7] in which assuming that

- the real vector field $f(y)$ of (1) is analytic and there is a compact set $\mathcal{K} \subset \mathbf{R}^m$ and constants K and $R > 0$ such that

$$\sup\{\|f(x)\|; x \in B_R(\mathcal{K})\} \leq K,$$

  where $B_r(\mathcal{K}) = \bigcup_{x_0 \in \mathcal{K}} B(x_0, R)$.

- ϕ_h is a real analytic map and there exists constant $M > K$ such that

$$\sup_{x \in B_{\alpha r}(\mathcal{K})} \|\phi_h(x) - x\| \leq (1-\alpha)M, \quad \text{for} \quad h < (1-\alpha)R/M,$$

  (This assumption is satisfied for all Runge–Kutta methods)

then there exist some $h_0 > 0$, $N = N(h)$ and constants C and M such that

$$\sup_{x \in \mathcal{K}} \|\phi_h(x) - \Phi_{h,\widetilde{f}_N}(x)\| \leq C\, h\, M\, e^{-p}\, e^{-\gamma/h},$$

where p is the order of the method and γ some constant.

Therefore, by taking a suitable number of terms in (8), the numerical flow of the truncated modified equation is exponentially convergent. The above analysis indicates that the flow of the modified equations is close to the flow of the numerical method in exponentially long intervals and therefore a comparison of the properties of the original and the modified equations provides a very convenient tool to study the qualitative properties of numerical methods.

If the vector field f of (1) belongs to a certain linear subspace $\mathcal{G}$ of the Lie algebra of smooth vector fields on $\mathbf{R}^m$ and the numerical method ϕ_h is a geometric integrator for this subspace for all $h \geq 0$ sufficiently small then it can be proved [7] that all modified vector fields $\widetilde{f}_i \in \mathcal{G}$. In particular if $\mathcal{G}$ is the linear subspace of Hamiltonian vector fields i.e. $f(y) = J^{-1}\, \nabla_y H(y)$ with $H : \mathbf{R}^{2d} \to \mathbf{R}$ sufficiently smooth and the numerical method ϕ_h is symplectic (observe that the diffeomorphisms that preserve the Hamiltonian form are the symplectic ones) then all modified vector fields $\widetilde{f}_i(y; h)$, $i = 1, 2, \ldots$ are also Hamiltonian, i.e. there exist $H_j : \mathbf{R}^{2d} \to \mathbf{R}$ such that $W_j = J^{-1}(H_j)_y$ and therefore

$$\widetilde{f}_i(y; h) = J^{-1}\, \nabla_y \left(\sum_{j=1}^{i} h^{j-1} H_j \right).$$

Similar remarks hold for other linear subspaces. Thus if $\mathcal{G}$ are the vector fields that preserve a particular first integral $F : \mathbf{R}^m \to \mathbf{R}$, i.e. $\partial_x F \cdot f = 0$ and ϕ_h is a geometric integrator for the F–preservation, $F \cdot \phi_h = F$ then the modified vector fields $\widetilde{f}_i$ preserve the first integral F ($\partial_x F \cdot \widetilde{f}_i = 0$).

3 Near Identity Transformations in The Lie-Hori Perturbation Theory

Hori's perturbation theory constructs near identity transformations $x \in \mathbf{R}^m \to y = \phi(x;\varepsilon) \in \mathbf{R}^m$ where $\varepsilon \in [0, \varepsilon_0]$ is a small parameter and $\phi(x; 0) = x$, that are defined as the solution $y(\tau) = y(\tau; \varepsilon, x)$ of an autonomous IVP with the form

$$\frac{dy(\tau)}{d\tau} = W(y(\tau); \varepsilon), \qquad y(0) = x \in \mathbf{R}^m, \tag{9}$$

for $\tau = \varepsilon$, i.e. $\phi(x;\varepsilon) = y(\varepsilon; \varepsilon, x)$. Here $W : \mathbf{R}^m \times [0, \varepsilon_0] \to \mathbf{R}^m$ is a sufficiently smooth vector function that is given as a power series expansion in the small parameter ε in the form

$$W(y;\varepsilon) = \sum_{j\geq 0} \frac{\varepsilon^j}{j!} W_{j+1}(y). \tag{10}$$

Such a function is usually called the (vector field) generating function of the near identity map $\phi(x;\varepsilon)$. Thus, for a given $\varepsilon > 0$, φ is the time– ε flow map of the autonomous differential equation (9). Equivalently, some authors (Reich [7]) describe ϕ as the time–one flow map of the vector field $\varepsilon W(y;\varepsilon)$.

In the context of Celestial Mechanics such a near identity maps (and also their generating functions W) are usually determined so that a given perturbed problem described by a set of non integrable differential equations is transformed into another set of equations whose flow can be studied more easily.

The main drawback of Hori's transformations (in contrast with Lie–Deprit [2] transformation) is that they do not satisfy the so called commutation theorem. However if we want to compute a repeated application of an Hori's transformation $\phi_\varepsilon(x) = y(\varepsilon; \varepsilon, x)$ associated to (9), since it is an autonomous system we have

$$\phi_\varepsilon^2(x) = \phi_\varepsilon(\phi_\varepsilon(x)) = y(\varepsilon; \varepsilon; \phi_\varepsilon(x)) = y(\varepsilon; \varepsilon, y(\varepsilon; \varepsilon, x)\ ) = y(\varepsilon + \varepsilon; \varepsilon, x),$$

and in general

$$\phi_\varepsilon^N(x) = y(N\varepsilon; \varepsilon, x),$$

i.e. the Nth power of ϕ_ε can be obtained as the solution of IVP (9) for the time $\tau = N\varepsilon$.

In view of this property if we have a numerical method that applied to (1) gives $y_{n+1} = \phi_h(y_n), n = 0, 1, \ldots$ we may consider the step size h as the small parameter ε and the continuous solution of IVP (1) $y(\tau; h, y_0)$ satisfies

$$y_n = \phi_h^n(y_0) = y(nh; h, y_0), \tag{11}$$

and therefore (9) will be the modified equations of the method ϕ_h applied to (1). This means that some techniques used in Hori's perturbation theory can be used to construct the modified equations of some numerical methods.

Next, let us revise some basic algorithms used in Hori's theory. Assuming that the generating function $W(x;\varepsilon)$ has the power series representation (10) we will derive recursively the functions $\varphi^{(j)}(x)$ of

$$y = \phi(x;\varepsilon) = x + \sum_{j\geq 1} \frac{\varepsilon^j}{j!}\varphi^{(j)}(x), \tag{12}$$

For $p = 1, 2, \ldots$ we denote the derivatives of the solution $y(\tau;\varepsilon,x)$ of (9) in the form

$$\frac{\partial^p y(\tau;\varepsilon,x)}{\partial\tau^p} = \sum_{j\geq 0} \frac{\varepsilon^j}{j!} W_{j+1}^{(p)}(y(\tau;\varepsilon,x)). \tag{13}$$

Clearly for $p = 1$

$$W_{j+1}^{(1)}(y) = W_{j+1}(y), \qquad j = 0, 1, \ldots \tag{14}$$

Next we introduce the Lie derivative of a tensor $\psi(x)$ along a vector field $W : \mathbf{R}^m \to \mathbf{R}$ which is an essential tool to describe the perturbation theories and allows us to give a clearly defined iterative procedure to compute the modified equations. Let $\Phi_{t,W}$ be the flow map of the vector field W, the Lie derivative of ψ along W is defined by

$$\mathcal{L}_W\psi(x) = \frac{d}{dt}\,\psi\left(\Phi_{t,W}(x)\right)\Big|_{t=0},$$

and represents the derivative of ψ in the direction of the vector field W. If $\psi : \mathbf{R}^m \to \mathbf{R}^m$ is a smooth vector field, the Lie derivatives $\mathcal{L}_s$ associated to the terms $W_s^{(1)}(y)$ of the vector field $W(y;\varepsilon)$ will be denoted by

$$\mathcal{L}_s\psi(y) = (\partial_y\ \psi(y))\ W_s^{(1)}(y), \qquad s = 1, 2, \ldots \tag{15}$$

where $\partial_y\psi$ is the Jacobian matrix.

It is easy to see that $W_j^{(p)}$ may be computed recursively by

$$W_{j+1}^{(p)} = \sum_{l=0}^{j} \binom{j}{l}\ \mathcal{L}_{j-l+1}W_{l+1}^{(p-1)}. \tag{16}$$

The computation of $W_j^{(p)}$ proceeds recursively according to the following table (referred to as the W–table):

$$\begin{array}{ccccccccc}
W_1^{(1)} & & & & & & & & \\
& \searrow & & & & & & & \\
W_2^{(1)} & & W_1^{(2)} & & & & & & \\
& \searrow & & \searrow & & & & & \\
W_3^{(1)} & & W_2^{(2)} & & W_1^{(3)} & & & & \\
& \searrow & & \searrow & & \searrow & & & \\
W_4^{(1)} & & W_3^{(2)} & & W_2^{(3)} & & W_1^{(4)} & & \\
& \searrow & & \searrow & & \searrow & & \searrow & \\
W_5^{(1)} & & W_4^{(2)} & & W_3^{(3)} & & W_2^{(4)} & & W_1^{(5)}
\end{array}$$

Given the elements $W_j^{(1)}, j = 1, \dots$ of the first column we compute recursively the elements of the second, third, etc rows. Thus in the first four rows we have

$$
\begin{array}{lcl}
\hline
W_1^{(2)} & = & \mathcal{L}_1 W_1^{(1)} \\
\hline
W_2^{(2)} & = & \binom{1}{0}\mathcal{L}_2 W_1^{(1)} + \binom{1}{1}\mathcal{L}_1 W_2^{(1)} \\
W_1^{(3)} & = & \mathcal{L}_1 W_1^{(2)} \\
\hline
W_3^{(2)} & = & \binom{2}{0}\mathcal{L}_3 W_1^{(1)} + \binom{2}{1}\mathcal{L}_2 W_2^{(1)} + \binom{2}{2}\mathcal{L}_1 W_3^{(1)} \\
W_2^{(3)} & = & \binom{1}{0}\mathcal{L}_2 W_1^{(2)} + \binom{1}{1}\mathcal{L}_1 W_2^{(2)} \\
W_1^{(4)} & = & \mathcal{L}_1 W_1^{(3)} \\
\hline
\end{array}
$$

According to (9),(10) Taylor's expansion of $y(\tau;\varepsilon,x)$ at $\tau = 0$ becomes

$$
\begin{aligned}
y(\tau;\varepsilon,x) &= y(0;\varepsilon,x) + \sum_{k\geq 1} \frac{\tau^k}{k!} \left.\frac{\partial^k y(\tau;\varepsilon,x)}{\partial \tau^k}\right|_{\tau=0} \\
&= x + \sum_{k\geq 1} \frac{\tau^k}{k!} \left(\sum_{j\geq 0} \frac{\varepsilon^j}{j!}\, W_{j+1}^{(k)}(x) \right)
\end{aligned}
$$

and putting $\tau = \varepsilon$ we get

$$
y(\varepsilon;\varepsilon,x) = x + \sum_{k\geq 1}\sum_{j\geq 0} \frac{\varepsilon^{k+j}}{k!j!} W_{j+1}^{(k)}(x) = x + \sum_{n\geq 1} \frac{\varepsilon^n}{n!} \sum_{k=1}^{n} \binom{n}{k}\, W_{n-k+1}^{(k)}(x),
$$

and comparing to (12) we get

$$
\varphi^{(n)} = \sum_{k=1}^{n} \binom{n}{k} W_{n-k+1}^{(k)}. \tag{17}
$$

Here $\varphi^{(n)}$ is given as a linear combination of the functions W that appear in the nth row of the above table. In the first orders we have

$$
\begin{aligned}
\varphi^{(1)} &= W_1^{(1)}, \\
\varphi^{(2)} &= \binom{2}{1} W_2^{(1)} + W_1^{(2)}, \\
\varphi^{(3)} &= \binom{3}{1} W_3^{(1)} + \binom{3}{2} W_2^{(2)} + W_1^{(3)}, \\
\varphi^{(4)} &= \binom{4}{1} W_4^{(1)} + \binom{4}{2} W_3^{(2)} + \binom{4}{3} W_2^{(3)} + W_1^{(4)}.
\end{aligned}
$$

Equations (16) and (17) allow us to determine recursively the near identity transformation associated to a given generating function W. Conversely, for a given near identity map (12) we may compute recursively the generating functions $W_j^{(1)}, j \geq 1$ by using again (17) and (16).

Consider now the case that the near identity map ϕ coincides with the Taylor expansion of the solution of $y' = f(y), y(0) = x$ at $t = \varepsilon$ up to some order $p \geq 1$, i.e.

$$\varphi^{(1)}(x) = f(x), \quad \varphi^{(2)}(x) = f'(f) = \mathcal{L}_f(f), \ldots, \varphi^{(p)}(x) = \mathcal{L}_f^{p-1}(f),$$

and $\varphi^{(p+1)}(x) \neq \mathcal{L}_f^p(f)$. Then it can be seen that all elements of the above W-table under the main diagonal up to the row p vanish identically and

$$W_1^{(1)} = f, \; W_1^{(2)} = \mathcal{L}_f(f), \; \ldots W_1^{(p)} = \mathcal{L}_f^{(p-1)}(f),$$

where $\mathcal{L}_1$ has been substituted by $\mathcal{L}_f$ and $W_1^{(1)}$ by f. This implies that the W–generating function (10) of the modified equation has the form

$$W(y;\varepsilon) = f(y) + \sum_{j \geq p} \frac{\varepsilon^j}{j!} W_{j+1}^{(1)}. \tag{18}$$

Further, in the rows $(p+1)$ and $(p+2)$ of the W–table the only non vanishing elements are

$$\begin{array}{cccccc} W_{p+1}^{(1)}, & 0, & \ldots & 0, & W_1^{(p+1)} & \\ W_{p+2}^{(1)}, & W_{p+1}^{(2)}, & \ldots & 0, & 0, & W_1^{(p+2)} \end{array}$$

Since $W_1^{(p+1)} = \mathcal{L}_f^p W_1^{(1)} = \mathcal{L}_f^p(f)$ and

$$\varphi^{(p+1)} = \binom{p+1}{1} W_{p+1}^{(1)} + \binom{p+1}{p+1} W_1^{(p+1)},$$

the first non vanishing term $W_{p+1}^{(1)}$ (after f) of the modified equation is given by

$$W_{p+1}^{(1)} = \binom{p+1}{1}^{-1} \left[\varphi^{(p+1)} - \mathcal{L}_f^p(f)\right]. \tag{19}$$

Observe that in view of (11) $\left[\varphi^{(p+1)}(x) - \mathcal{L}_f^p(f)\right] \varepsilon^{p+1}/(p+1)!$ is the leading term of the local error of the ϕ–method.

Next, since

$$W_{p+1}^{(2)} = \binom{p}{0} \mathcal{L}_{p+1} W_1^{(1)} + \binom{p}{p} \mathcal{L}_1 W_{p+1}^{(1)} = \mathcal{L}_{p+1}(f) + \mathcal{L}_f W_{p+1}^{(1)},$$

and $W_1^{(p+2)} = \mathcal{L}_f^{p+1}(f)$, it follows from

$$\varphi^{(p+2)} = \binom{p+2}{1} W_{p+2}^{(1)} + \binom{p+2}{2} W_{p+1}^{(2)} + \binom{p+2}{p+2} W_1^{(p+2)},$$

that the second non vanishing term is given by

$$W_{p+2}^{(1)} = \binom{p+2}{1}^{-1} \left[\varphi^{(p+2)} - \mathcal{L}_f^{p+1}(f) - \binom{p+2}{2} \left(\mathcal{L}_{p+1} W_1^{(1)} + \mathcal{L}_1 W_{p+1}^{(1)}\right)\right]. \tag{20}$$

Note that these terms can be easily derived by using the inverse of (12).

4 Some Examples and Applications

For the sake of brevity we include here only one example. We consider the differential equation of the simple pendulum as an example of non linear undamped oscillation that is solved by means of the fourth order Runge–Kutta method defined by the Butcher array

$$\begin{array}{c|cccc} 0 & & & & \\ 1/2 & 1/2 & & & \\ 1/2 & 0 & 1/2 & & \\ 1 & 0 & 0 & 1 & \\ \hline & 1/6 & 2/6 & 2/6 & 1/6 \end{array} \tag{21}$$

whose equations are

$$y_{n+1} = y_n + h\sum_{i=1}^{4} b_i f_i, \quad \text{with} \quad f_i = f\left(y_n + h\sum_{j=1}^{i-1} a_{ij} y_j\right)$$

The second order equation of pendulum $q'' = -\sin(q)$ is written as a set of two first order equations

$$y' = \begin{pmatrix} p \\ q \end{pmatrix}' = f(y) = \begin{pmatrix} -\sin(q) \\ p \end{pmatrix}. \tag{22}$$

Denoting by $\phi_{h,f}$ the numerical h–flow map and by $\Phi_{t,f}$ the exact flow map, after some calculation it is found that

$$\phi_{h,f}(y) - \Phi_{h,f}(y) = \frac{h^5}{5!}\xi_5(y) + \ldots$$

with $\xi_5 = \xi_5(p,q) \in \mathbf{R}^2$ given by

$$\xi_5 = \frac{-1}{4!}\begin{pmatrix} \sin q(-21 + p^4 + 36p^2\cos q - 3\cos(2q) \\ 2p(3 + 2p^2\cos q + 9\cos(2q) \end{pmatrix},$$

since $\xi_5 \not\equiv 0$ the numerical method has indeed order four for this equation.

Next we compute the first two perturbation terms of the modified equations. Consistently with the above notations we write the modified equations in the form

$$\tilde{y}' = f(\tilde{y}) + \frac{h^4}{4!}W_5^{(1)}(\tilde{y}) + \frac{h^5}{5!}W_6^{(1)}(\tilde{y}) + \ldots \tag{23}$$

where according to (19), $W_5^{(1)}$ is given by

$$W_5^{(1)} = \frac{1}{5}\xi_5 = \frac{-1}{5!}\begin{pmatrix} \sin q\,(-21 + p^4 + 36p^2\cos q - 3\cos(2q)) \\ 2p\,(3 + 2p^2\cos q + 9\cos(2q) \end{pmatrix}. \tag{24}$$

Next by using (20) we get for the following term of the modified equation

$$W_6^{(1)} = \frac{1}{48}\begin{pmatrix} 5p\,(-2p^2 - 9\cos q + \cos(3q)) \\ 5(p^2 - 4\cos q)\sin(2q) \end{pmatrix}. \tag{25}$$

Let us see that a study of the modified equation (23),(22),(24),(25) may give some insight on the behaviour of the numerical method.

The original problem (22) is Hamiltonian with $H = (1/2)p^2 - \cos q$, however the numerical method RK4 is not symplectic and therefore we do not expect ϕ_{hf} to be symplectic. Nevertheless in this case it is easy to check that $\text{div } W_5^{(1)} = 0, \quad \text{div } W_6^{(1)} \neq 0$ and therefore the modified system with the first perturbation term is Hamiltonian with

$$\widetilde{H}(y;h) = \frac{1}{2}p^2 - \cos q - \frac{h^4}{4!\ 240}\Big(6p^2 + 2p^4\cos q + 18p^2\cos(2q) - 39\cos q - \cos(3q)\Big).$$

Now the numerical solution remains in exponentially long time intervals into the constant energy manifold $\widetilde{H}(y;h) = \widetilde{C}$.

Given the initial conditions $p_0 = 0, q_0 = \alpha > 0$ (corresponding to an oscillating solution), it is well known that in the original problem the pendulum describes the curve

$$p = \pm\sqrt{2(-\cos\alpha + \cos q)}, \qquad q \in [-\alpha, \alpha]$$

with period

$$T = 4\int_0^{\pi/2}\Big(1 - \sin^2(\alpha/2)\ \sin^2 u\Big)^{-1/2}\ du.$$

In the first order modified equations with the same initial conditions the solution describes (for small $|\gamma|$ with $\gamma = -h^4/(4!\ 120)$)

$$p = \pm\sqrt{\frac{-2C}{\sqrt{B^2 - 4AC} + B}}, \qquad q \in [-\alpha, \alpha],$$

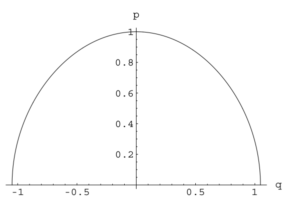
where

$$\begin{aligned} A &= 2\gamma\cos q, \qquad B = (1/2) + 6\gamma + 18\gamma\cos(2q), \\ C &= -(1+29\gamma)\cos q - \gamma\cos(3q) + (1+39\gamma)\cos\alpha + \gamma\cos(3\alpha), \end{aligned}$$

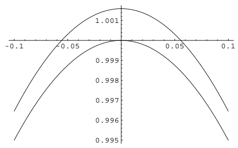
due to the fact that $-2C \geq 0$ for all $q \in [-\alpha, +\alpha]$ but $-2C < 0$ outside this interval.

Further the motion in the perturbed manifold $\widetilde{H} = \widetilde{C}$ is also periodic with a period $\widetilde{T} > T$ (the expression of $\widetilde{T}$ is too complicated).

The figure of the (upper) perturbed and unperturbed orbits corresponding to the initial conditions $p_0 = 0, q_0 = \alpha = \pi/3$ is displayed for $q \in [-\alpha, +\alpha]$ in the phase plane (q,p).



Since they are very close, at first sight the figure is the same but for $q \simeq 0$ the non perturbed orbit is under the perturbed one as shown in the following figure



The two orbits coincide at both ends of the interval $[-\alpha, +\alpha]$ and cross at $q = \pm 0.359025$.

A complete study of the relative graphs and periods of these orbits can be carried out for all kind of orbits.

The above remarks show how the BEA together with the Lie–Hori perturbation theory can be used to analyze the behaviour of the one step methods for a given problem. Here a first order perturbation theory permits to describe the Hamiltonian behaviour of the method for this problem, however higher order terms do not retain this symplectic behaviour.

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