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Symplectic integration of Hamiltonian systems using polynomial maps

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Abstract

In order to perform numerical studies of long-term stability in nonlinear Hamiltonian systems, one needs a numerical integration algorithm which is symplectic. Further, this algorithm should be fast and accurate. In this Letter, we propose such a symplectic integration algorithm using polynomial map refactorization of the symplectic map representing the Hamiltonian system. This method should be particularly useful in long-term stability studies of particle storage rings in accelerators.

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1. Introduction

Long-term single particle stability studies of particle storage rings play an important role in the design of accelerators [1]. These storage rings are generally described by nonlinear, nonintegrable Hamiltonians. Therefore analytical results on long-term stability of particle motion in such storage rings are difficult to obtain. By default, numerical integration of particle trajectories is the primary tool used to explore the dynamics of these systems. However, standard numerical integration algorithms cannot be used since they are not symplectic [2]. This violation of the symplectic condition can lead to spurious chaotic or dissipative behavior. Numerical integration algorithms which satisfy the symplectic condition are called symplectic integration algorithms [3].

Several symplectic integration algorithms have been proposed in the literature [4]. Some of these directly use the Hamiltonian whereas others use the symplectic map [2] representing either the entire storage ring (in which case one obtains the so-called one-turn map) or major segments of the ring. For complicated systems like the Large Hadron Collider which has thousands of elements, using individual Hamiltonians for each element can drastically slow down the integration process. On the other hand, the map based approach is very fast in such cases [5]. Further, if nonlinearities in the symplectic map are too "large", one can use scaling and squaring techniques [6] to alleviate the problem.

One class of the map-based methods uses jolt factorization [7,8]. But there are still unanswered questions on how to best choose the underlying group and elements in the group [9]. Further, some of these methods [8] can be quite difficult to generalize to higher dimensions. Another class of methods uses solvable

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maps [10] or monomial maps [11]. Even though they are fairly straightforward to generalize to higher dimensions, they tend to introduce spurious poles and branch points not present in the original map [9].

In this Letter, we propose a new symplectic integration method where the symplectic map is refactorized using "polynomial maps" (maps whose action on phase space variables gives rise to polynomials). This does not introduce spurious poles and branch points. Moreover, it is easy to generalize to higher dimensions. In this Letter, we restrict ourselves to maps in six-dimensional phase space which are appropriate for single particle stability studies. We show that the method gives good results. Further, since it is map-based, it is also very fast.

2. Preliminaries

We start by representing a Hamiltonian system by a symplectic map [2]. For simplicity we restrict ourselves to a six-dimensional phase space. Let us denote the collection of six phase-space variables q_i, p_i $(i = 1, 2, 3)$ by the symbol z:

$$z = (q_1, q_2, q_3, p_1, p_2, p_3). \tag{1}$$

The Lie operator [2] corresponding to a phase-space function $f(z)$ is denoted by $:f(z):$. It is defined by its action on a phase-space function $g(z)$ as shown below:

$$:f(z):g(z) = \big[f(z), g(z)\big]. \tag{2}$$

Here $[f(z), g(z)]$ denotes the usual Poisson bracket of the functions $f(z)$ and $g(z)$. Next, we define the exponential of a Lie operator. It is called a Lie transformation [2] and is given as follows:

$$e^{:f(z):} = \sum_{n=0}^{\infty} \frac{:f(z):^n}{n!}. \tag{3}$$

The effect of a Hamiltonian system on a particle can be formally expressed as the action of a map $\mathcal{M}$ that takes the particle from its initial state z^{in} to its final state z^{fin}:

$$z^{\mathrm{fin}} = \mathcal{M} z^{\mathrm{in}}. \tag{4}$$

It can be shown that $\mathcal{M}$ is a symplectic map [2]. Consider its Jacobian matrix which we denote by M. Symplectic maps are maps whose Jacobian matrices M satisfy the following "symplectic condition":

$$\tilde{M} J M = J, \tag{5}$$

where $\tilde{M}$ is the transpose of M and J is the fundamental symplectic matrix.

Using the Dragt–Finn factorization theorem [2,12], the symplectic map $\mathcal{M}$ can be factorized as shown below:

$$\mathcal{M} = \hat{M} e^{:f_3:} e^{:f_4:} \dots e^{:f_n:} \dots. \tag{6}$$

Here $f_n(z)$ denotes a homogeneous polynomial (in z) of degree n uniquely determined by the factorization theorem. Further $\hat{M}$ gives the linear part of the map and hence has an equivalent representation in terms of the Jacobian matrix M of the map $\mathcal{M}$ [2]:

$$\hat{M} z_i = M_{ij} z_j = (Mz)_i. \tag{7}$$

The infinite product of Lie transformations $\exp(:f_n:)$ $(n = 3, 4, \dots)$ in Eq. (6) represents the nonlinear part of $\mathcal{M}$.

Using the above procedure, one can represent each element in the storage ring by a symplectic map. By concatenating [2] these maps together, we obtain the so-called "one-turn" map representing the entire storage ring. This concatenation is made possible by the Campbell–Baker–Hausdorff (CBH) theorem [13]. The one-turn map gives the final state $z^{(1)}$ of a particle after one turn around the ring as a function of its initial state $z^{(0)}$:

$$z^{(1)} = \mathcal{M} z^{(0)}. \tag{8}$$

To obtain the state of a particle after N turns, one has to merely iterate the above mapping N times, i.e.,

$$z^{(N)} = \mathcal{M}^n z^{(0)}. \tag{9}$$

Since $\mathcal{M}$ is explicitly symplectic, this gives a symplectic integration algorithm. Further, since the entire ring can be represented by a single (or at most a few) symplectic map(s), numerical integration of particle trajectories using symplectic maps is very fast.

3. Symplectic integration using polynomial maps

It is obvious that one cannot use $\mathcal{M}$ in the form given in Eq. (6) for any practical computations. It involves an infinite number of Lie transformations.

Therefore, we have to truncate $\mathcal{M}$ by stopping after a finite number of Lie transformations:

$$\mathcal{M} \approx \hat{M} e^{:f_3:} e^{:f_4:} \ldots e^{:f_P:}. \tag{10}$$

However, each exponential $e^{:f_n:}$ in $\mathcal{M}$ still contains an infinite number of terms in its Taylor series expansion. One possible solution is to truncate the Taylor series generated by the Lie transformations to order P. But this violates the symplectic condition.

We get around the above problem by refactorizing $\mathcal{M}$ in terms of simpler symplectic maps which can be evaluated exactly without truncation. We use "polynomial maps" which give rise to polynomials when acting on the phase space variables. This avoids the problem of spurious poles and branch points present in generating function methods [9], solvable map [10] and monomial map [11] refactorizations. To determine which symplectic maps give rise to polynomial mappings, consider $\exp(:h(z):)$, where $h(z)$ is a polynomial. Since all Lie transformations are symplectic maps [2], this is a symplectic map. Its action on phase space variables is equivalent to solving the Hamilton's equations of motion from time $t = 0$ to $t = -1$ using $h(z)$ as the Hamiltonian. For example, consider the action of $\exp(:q_1^3:)$ on q_1, p_1 in a two-dimensional phase space. We first solve the following Hamilton's equations of motion:

$$\frac{dq_1}{dt} = \frac{\partial h}{\partial p_1}, \qquad \frac{dp_1}{dt} = -\frac{\partial h}{\partial q_1}, \tag{11}$$

with $h = q_1^3$. Solving these simple equations, we obtain

$$q_1(t) = q_1(0), \qquad p_1(t) = p_1(0) - 3q_1(0)^2 t, \tag{12}$$

where $q_1(0)$ and $p_1(0)$ denote the values of q_1 and p_1 at time $t = 0$. To obtain the action of the map $\exp(:q_1^3:)$ on the phase space variables, set $t = -1$ in the above equations and denote $q_1(-1)$, $p_1(-1)$ by q_1^{fin}, p_1^{fin} and $q_1(0)$, $p_1(-0)$ by q_1^{in}, p_1^{in}, respectively. Thus we get

$$q_1^{\text{fin}} = q_1^{\text{in}}, \qquad p_1^{\text{fin}} = p_1^{\text{in}} + 3\big(q_1^{\text{in}}\big)^2. \tag{13}$$

Using Eq. (3), we can easily verify that the above result is indeed correct.

Using the above procedure, we can identify symplectic maps $\exp(:h(z):)$ which give rise to polynomial mappings of the phase space variables into themselves. These results [14] can be codified as the following simple principles which are easily generalized to higher dimensions also:

1. All polynomials of the form $h(z)$ where both a phase space variable and its canonically conjugate variable [15] do not occur simultaneously give rise to polynomial symplectic maps via $\exp(:h(z):)$.
2. If a canonically conjugate pair $\{q_i, p_i\}$ is present in the polynomial $h(z)$, it only appears either in the form $a(z')q_i + g(p_i, z')$ or $a(z')p_i + g(q_i, z')$ or its integer powers. Here z' denotes the collection of phase space variables $\{q_j, p_k\}$ with $j \neq k \neq i$. Further, a and g are polynomials in the indicated variables.

We now return to the problem of symplectic integration. For the present, we restrict ourselves to one-turn symplectic maps in a two-dimensional phase space truncated at order 4. The results obtained below can be generalized to higher orders using symbolic manipulation programs. The Dragt–Finn factorization of the symplectic map is given by

$$\mathcal{M} = \hat{M} e^{:f_3:} e^{:f_4:}, \tag{14}$$

where

$$\begin{aligned} f_3 &= a_1 q_1^3 + a_2 q_1^2 p_1 + a_3 q_1 p_1^2 + a_4 p_1^3, \\ f_4 &= a_5 q_1^4 + a_6 q_1^3 p_1 + a_7 q_1^2 p_1^2 + a_8 q_1 p_1^3 + a_9 p_1^4. \end{aligned} \tag{15}$$

Here the coefficients $a_1, \ldots, a_9$ can be explicitly computed given a Hamiltonian system [2]. The above map captures the leading-order nonlinearities of the system. Since the action of the linear part $\hat{M}$ on phase space variables is well known (cf. Eq. (7)) and is already a polynomial action, we only refactorize the nonlinear part of map using polynomial maps. It turns out that we require 7 polynomial maps for this purpose:

$$\mathcal{M} \approx \mathcal{P} = \hat{M} e^{:h_1:} e^{:h_2:} \ldots e^{:h_7:}, \tag{16}$$

where the numeral appearing in the subscript indexes the polynomial maps. The h_i's are given as follows:

$$\begin{aligned} h_1 &= b_1 q_1^3 + b_5 q_1^4, \\ h_2 &= b_4 p_1^3 + b_9 p_1^4, \\ h_3 &= (b_2 + b_3)(q_1 + p_1)^3, \\ h_4 &= (b_3 - b_2)(q_1 - p_1)^3, \\ h_5 &= \big(q_1 + p_1 + b_8 p_1^2\big)^3, \end{aligned}$$

$$h_6 = \left(-q_1 - p_1 + b_6 q_1^2\right)^3,$$
$$h_7 = b_7 (q_1 + p_1)^4. \tag{17}$$

Here b_i's are at present unknown coefficients. By forcing the refactorized form $\mathcal{P}$ to equal the original map $\mathcal{M}$ up to order 4 and using the CBH theorem [13], we can easily compute these unknown coefficients in terms of the known a_i's. These expressions are given in the Appendix. The explicit actions of the polynomial maps on the phase space variables are also given there. This completely determines the refactorized map $\mathcal{P}$. Each $\exp(:h_i:)$ is a polynomial map which can be evaluated exactly and is explicitly symplectic. Thus by using $\mathcal{P}$ instead of $\mathcal{M}$ in Eq. (9), we obtain an explicitly symplectic integration algorithm. Further, it is fast to evaluate and does not introduce spurious poles and branch points. The above factorization is not unique. However, the principles outlined earlier impose restrictions on the possible forms and this eases considerably the task of refactorization. Moreover, we require the coefficients b_i to be polynomials in the known coefficients a_i. Otherwise this can lead to divergences when a_i's take on certain special values. Finally, we minimize the number of polynomial maps in the refactorized form. Our studies show that different polynomial map refactorizations obeying the above restrictions do not lead to any significant differences in their behavior.

The above refactorization has also been extended to symplectic maps in a six-dimensional phase space truncated at order 4. In this case, we require 23 polynomial maps in the refactorization to make $\mathcal{P}$ equal to $\mathcal{M}$ up to order 4:

$$\mathcal{M} \approx \mathcal{P} = \hat{M} e^{:h_1:} e^{:h_2:} \ldots e^{:h_{23}:}, \tag{18}$$

where the numeral appearing in the subscript indexes the polynomial maps. Since listing out the explicit forms of the h_i's and their coefficients is not particularly illuminating, we do not list them here. However, a FORTRAN program which implements the above polynomial map refactorization is available from the author upon request.

We now analyze the leading-order error committed in our method. In our method, we first truncate the symplectic map to a given order and then refactorize it using a product of polynomial maps. Both these stages give rise to errors. When we truncate the symplectic map $\mathcal{M}$ at the nth order, we obtain

$$\mathcal{M}_n = \hat{M} \exp(:f_3:) \exp(:f_4:) \ldots \exp(:f_n:). \tag{19}$$

The leading term that has been omitted is $\exp(:f_{n+1}:)$. From properties of Lie transformations and Lie operators [2], we have

$$\exp(:f_{n+1}:) z = z + [f_{n+1}, z] + \cdots, \tag{20}$$

where $[\,,]$ denotes the usual Poisson bracket. Now, $[f_{n+1}, z]$ gives terms of the form z^n [2]. Thus error due to truncation of the symplectic map is of order z^n.

Next, we refactorize the truncated symplectic map $\mathcal{M}_n$ as a product of k polynomial maps:

$$\mathcal{M}_n = \hat{M} \exp(:h_1:) \exp(:h_2:) \ldots \exp(:h_k:). \tag{21}$$

These polynomial maps are obtained by first using the CBH series to combine the Lie transformations and then comparing with the original symplectic map. Both these maps are made to agree up to order n. Therefore, the leading error term is again of the form $\exp(:f_{n+1}:)$ giving rise to an error of order z^n.

4. Applications

We now consider two applications of the above method. The first example is to find the region of stability of the following simple symplectic map:

$$\mathcal{M} = \hat{M} \exp\left[:(q_1 + p_1)^3:\right], \tag{22}$$

where

$$\hat{M} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}, \tag{23}$$

and $\theta = \pi/3$. We chose this example since the exact action of the above map is known and hence the exact region of stability can also be determined. We found excellent agreement between results obtained using polynomial maps and the exact results.

We have also applied the method to more complicated Hamiltonian systems like particle storage rings. We studied an electron storage ring with radio frequency bunching cavities. The storage ring is composed of drifts, bending magnets, quadrupoles, sextupoles and RF cavities. The efficacy of our method is best revealed for such complicated Hamiltonian systems. Since there are many constituent elements (in

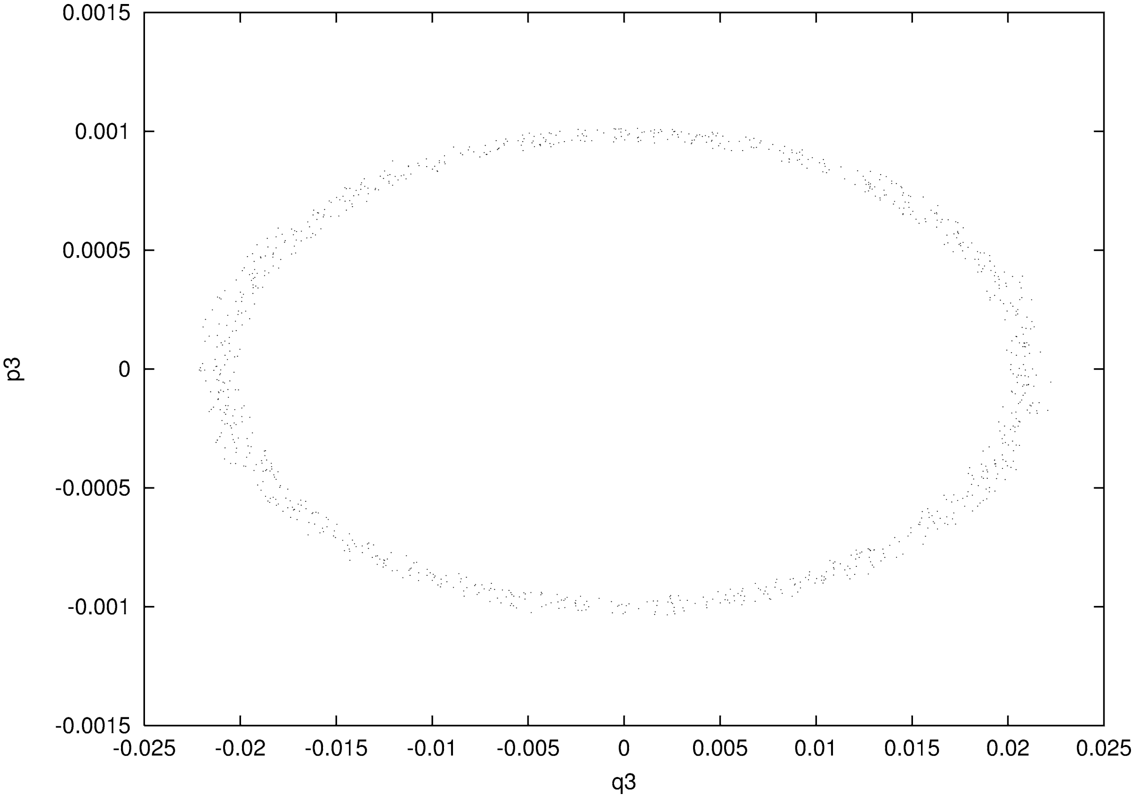

Fig. 1. This figure shows the q_3–p_3 phase space plot for one million turns around a storage ring using the polynomial map method (only every 1000th point is plotted).

storage rings like the Large Hadron Collider, there can be thousands of elements), numerical integration using Hamiltonians for each element is cumbersome and slow. On the other hand, a map based approach where one represents the entire storage ring in terms of a single map is much faster [5]. When this is combined with our polynomial map refactorization, one obtains a symplectic integration algorithm which is both fast and accurate and is ideally suited for such complex real life systems. The q_3–p_3 phase plot for one million turns around the ring using our polynomial map method is given in Fig. 1. In this case, q_3 and p_3 represent the deviations from the closed orbit time of flight and energy, respectively. From theoretical considerations, we expect the so-called synchrotron oscillations in these variables. This manifests itself as ellipses in the phase space plot of q_3 and p_3 variables (just as the oscillations of the simple pendulum manifest themselves as ellipses in the coordinate–momentum phase space plot). In Fig. 1, we observe the expected synchrotron oscillations.

5. Conclusions

To conclude, we have proposed a new symplectic integration algorithm based on polynomial map refactorization. This should be of help in studying long term stability of complicated accelerator systems and other Hamiltonian systems.

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Appendix

The coefficients b_i in Eq. (17) can be easily determined using the CBH theorem [13]. Their expressions in terms of the known coefficients a_i of the symplectic map $\mathcal{M}$ (cf. Eq. (15)) is given as follows:

$$\begin{aligned}
&b_1 = a_1 - a_3/3, \qquad b_2 = a_2/6,\\
&b_3 = a_3/6, \qquad b_4 = a_4 - a_2/3,\\
&b_6 = \big(2a_6 - 2a_7 + a_8 + 18b_1b_2 - 36b_2^2 - 36b_1b_3\\
&\qquad + 36b_3^2 + 9b_1b_4 + 18b_2b_4 - 18b_3b_4\big)/6,\\
&b_7 = \big(-a_6 + 2a_7 - a_8 - 18b_1b_2 + 36b_2^2 + 18b_1b_3\\
&\qquad - 36b_3^2 - 9b_1b_4 - 18b_2b_4 + 18b_3b_4\big)/4,\\
&b_8 = \big(a_6 - 2a_7 + 2a_8 + 18b_1b_2 - 36b_2^2 - 18b_1b_3\\
&\qquad + 36b_3^2 + 9b_1b_4 + 36b_2b_4 - 18b_3b_4\big)/6,\\
&b_5 = a_5 - 9b_1b_2 - 9b_2^2 + 9b_3^2 - 3b_6 - b_7,\\
&b_9 = a_9 - 9b_2^2 + 9b_3^2 + 9b_3b_4 - b_7 - 3b_8.
\end{aligned} \tag{24}$$

Note that the formulas have been sequenced in such a way that once a given b_i is evaluated, it is used in the formulas for the b_i's following it.

The actions of the polynomial maps $\exp(:h_i:)$ ($i = 1, 2, \ldots, 7$) on the phase space variables q_1, p_1 are easily evaluated using the procedure outlined in the main text (see the discussion before Eq. (11). We obtain the following results:

$$\begin{aligned}
&e^{:h_1:}q_1 = q_1, \qquad e^{:h_1:}p_1 = p_1 + 3b_1q_1^2 + 4b_5q_1^3,\\
&e^{:h_2:}q_1 = q_1 - 3b_4p_1^2 - 4b_9p_1^3, \qquad e^{:h_2:}p_1 = p_1,\\
&e^{:h_3:}q_1 = q_1 - 3(b_2 + b_3)(q_1 + p_1)^2,\\
&e^{:h_3:}p_1 = p_1 + 3(b_2 + b_3)(q_1 + p_1)^2,\\
&e^{:h_4:}q_1 = q_1 + 3(b_3 - b_2)(q_1 - p_1)^2,\\
&e^{:h_4:}p_1 = p_1 + 3(b_3 - b_2)(q_1 - p_1)^2,\\
&e^{:h_5:}q_1 = q_1 - c_1(1 + 2b_8p_1 + b_8c_1),\\
&e^{:h_5:}p_1 = p_1 + c_1,\\
&e^{:h_6:}q_1 = q_1 + c_2,\\
&e^{:h_6:}p_1 = p_1 - c_2(1 - 2b_6q_1 - b_6c_2),\\
&e^{:h_7:}q_1 = q_1 - 4b_7(q_1 + p_1)^3,\\
&e^{:h_7:}p_1 = p_1 + 4b_7(q_1 + p_1)^3,
\end{aligned} \tag{25}$$

where

$$\begin{aligned}
&c_1 = 3\big(q_1 + p_1 + b_8p_1^2\big)^2,\\
&c_2 = 3\big(-q_1 - p_1 + b_6p_1^2\big)^2.
\end{aligned} \tag{26}$$

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