PROBLEMS OF CONSERVATIVE INTEGRATION IN BEAM PHYSICS

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Abstract

In this paper an approach to conservative integration methods development is discussed. This problem is very important for beam physics: from beam line synthesis up to long time evolution simulation. This approach is based on a Lie algebra technique. On the first step we find a special form of decomposition for a Lie map, describing the system under study. On the second step a researcher finds exact solutions for some classes of hamiltonians in symbolic forms. These steps allows forming an integration scheme, which have a desired symplectic property. The additional invariant and symmetry properties can be included using dynamical invariants conception.

INTRODUCTION

Numerical integration algorithms play an essential role in investigation of the long term beam particle evolution, stability of similar process, nonlinear nonintegrable Hamiltonian systems. For example, as it is known, standard numerical integration methods are not symplectic and this violation of the symplectic condition can lead to some false effects, for example, spurious chaotic, dissipative behavior.

There are several approaches devoted to development of numerical methods preserving some qualitative structure, which inheres to the dynamical system under study. These schemes will be noted as conservative integration schemes. It is possible to distinguish the two following approaches: the first is based on correcting procedure for usual numerical methods for integration scheme (for example, for the well known Runge–Kutta scheme, [1]). The second one originates in solution description with the help of a map. This map has all requisite properties. But its numerical realization losses these properties, and it is necessary to ensure desired properties for a numerical variant of this map too. In this report we take after the second approach.

It is necessary to distinguish two types of integration schemes: "symplectic integration method" for numerical methods which satisfy the symplectic condition exactly and "pseudo-symplectic integration method" in the case, when the symplectic condition is fulfilled not exactly, but with some given accuracy. The exact symplectic schemes are main interest of this paper.

Several symplectic integration methods have been proposed in the literature (see, for example, [2, 3, 4]).

According to the notation of work [5] we will also distinguish two types of invariants: dynamical and kinematical ones. The kinematical invariants play the preferred role in the numerical integration problem because of they describe a class of dynamical systems. After ensuring kinematical invariant preservation one can passes to ensuring one or several dynamical invariants. Here there are several approaches. The very interesting method was published by V.I. Zubov [6]. He proposed to modify standard numerical integration methods using techniques of control theory. This approach allows generating some conservative numerical methods for any kind of invariants.

A concept of invariants allows to use the tools of symmetry theory permitting to write any invariant property as an appropriate symmetry condition [7].

In this paper we consider a problem of construction of symplectic integrators for an explicit symplectic map, generated by hamiltonian dynamical systems. It is well known that Lie algebraic methods have found applications in accelerator physics. These techniques demonstrate the advantage of guaranteeing explicit approximating systems that are also hamiltonian.

BEAM PROPAGATOR DECOMPOSITION

So, let us consider an initial problem for a system of ordinary differential equations for a phase vector of particles states $\mathbf{X}$:

$$\frac{d\mathbf{X}}{ds} = \mathbf{F}(\mathbf{X}, s) = \mathbb{J}\partial\mathcal{H}(\mathbf{X}, s)/\partial\mathbf{X}^*, \;\; \mathbf{X}(s_0) = \mathbf{X}_0, \quad (1)$$

where $\mathcal{H}(\mathbf{X}, s)$ is a hamiltonian described the system under study and $\mathbb{J}$ — a symplectic matrix. According to the Lie algebraic approach eq. (1) involves the following operator equation:

$$\frac{d\mathcal{M}(s|s_0)}{ds} = \mathcal{L}[\mathbf{F}] \circ \mathcal{M}(s|s_0), \;\; \mathcal{M}(s_0|s_0) = \mathcal{I}d, \quad (2)$$

where $\mathcal{L}[\mathbf{F}]$ is a Lie operator, associated with a vector function $\mathbf{F}$ ($\mathcal{L} = \mathbf{F}^*\partial/\partial\mathbf{X}$), $\mathcal{M}(s|s_0)$ is a Lie map, generated by eq. (1), or a beam propagator, and $\mathcal{I}d$ — the identical operator. In the literature there are several types of Lie map factorization (see, e.g. [8]). Let us consider a some another type of map factorization — a "propagator decomposition" of the following form

$$\mathcal{M} \approx \mathcal{M}^M = \mathcal{M}_M \circ \ldots \circ \mathcal{M}_1, \quad (3)$$

where $\mathcal{M}_k = \mathcal{M}[\mathcal{L}_k]$ ($k = \overline{1, M}$) is defined by some Lie operator $\mathcal{L}_k = \mathcal{L}_k[\mathbf{F}_k] = \mathbf{F}_k^*\partial/\partial\mathbf{X}$, associated with homogeneous polynomials $\mathbf{F}_k$ (or homogeneous hamiltonians $\mathcal{H}_k(\mathbf{X})$). The selection of these operators is defined

0-7803-8859-3/05/$20.00

according to the following condition:
Condition 1:
– *the initial problem for operator differential equations*

$$\frac{d\mathcal{M}_k}{ds} = \mathcal{L}_k \circ \mathcal{M}_k,\ \mathcal{M}_k(s_0|s_0) = \mathcal{I}d, \tag{4}$$

has a exact solution in some class of entire functions;
– *the approximation* (3) *for some M has a sufficient estimation*.

So we have two problems: the first — to define types of homogeneous polynomials $\mathbf{F}_k$, which allow to evaluate eq. (4) in a symbolic form, and the second — to determine an order of approximation M for these types of $\mathbf{F}_k$. The finite product $\mathcal{M}^M$ (see (3)) gives us a symplectic approximation for the solution of eq. (2).

Exact Solutions for Homogeneous Hamiltonians

The first mentioned problem can be solved according to the approach, developed in the paper [9]. Using this approach one can evaluate symbolic presentation for propagators for some homogeneous hamiltonians or functions as a right side of a differential equations system. Let us put $\mathbf{F}(\mathbf{X}, t) = \mathbb{P}_m(t)\mathbf{X}^{[m]}$, where the matrix $\mathbb{P}_m(t)$ has a special form. This form is bound up with the problem of symplectic factorization (see, e.g. [8, 10]).

Eq. (1) with homogeneous function $\mathbf{F}(\mathbf{X}, s)$ is solved as

$$\mathcal{M} \circ \mathbf{X}_0 = \mathbf{X}\left(\mathbf{X}_0; s\,|\,s_0\right) = \frac{\mathbf{P}_N\left(\mathbf{X}_0; s\,|\,s_0\right)}{Q_L\left(\mathbf{X}_0; s\,|\,s_0\right)}, \tag{5}$$

where $\mathbf{P}_N\left(\mathbf{X}_0; s\,|\,s_0\right)$ and $Q_L\left(\mathbf{X}_0; s\,|\,s_0\right)$ — vector and scalar polynomials of N- and L-order correspondingly:

$$\mathbf{P}_N\left(\mathbf{X}_0; s\,|\,s_0\right) = \sum_{k=0}^{N} \mathbb{P}^k(s\,|\,s_0)\mathbf{X}_0^{[k]},$$

$$Q_L\left(\mathbf{X}_0; s\,|\,s_0\right) = \sum_{j=0}^{L} \mathbf{Q}_j^*(s\,|\,s_0)\mathbf{X}_0^{[j]}.$$

Here $\mathbb{P}^k(s\,|\,s_0)$ and $\mathbf{Q}_j(\mathbf{X}_0; s\,|\,s_0)$ — matrix and scalar functional coefficients. Here we suggest that there is $Q_L \neq 0$ in an interesting domain of $\mathbf{X}_0$.

Let us consider $\mathcal{M} = \mathcal{M}_m = \exp\left((s - s_0)\mathcal{L}_m\right)$, where $\mathcal{L}_m = \mathbf{G}_m^*(\mathbf{X}_0)\partial/\partial\mathbf{X}_0$. Using the matrix formalism for Lie algebraic tools [11] one can write

$$\mathcal{M}_m \circ \mathbf{X}_0 = \mathbf{X}_0 + \sum_{k=1}^{\infty} \frac{(s - s_0)^k \mathbb{P}_m^{1k}}{k!} \mathbf{X}_0^{[k(m-1)+1]},$$

where $\mathbb{P}_m^{1k} = \prod_{j=1}^{k} \mathbb{G}_m^{\oplus((j-1)(m-1)+1)}$, and

$$\mathcal{M}_m \circ \mathbf{X}_0 = \sum_{k=0}^{\infty} \frac{(s - s_0)^k}{k!} \mathbb{P}_m^{1k} \mathbf{X}_0^{[k(m-1)+1]} = \\ = \sum_{l=0}^{N} \mathbb{P}_m^l \mathbf{X}_0^{[l]} \Big/ \sum_{j=0}^{L} \mathbf{Q}_j^* \mathbf{X}_0^{[j]}. \tag{6}$$

N o t a t i o n. Expression (6) is a an extension of Padé approximation for many-dimensional case.

So, we have

$$\sum_{k=0}^{\infty} \frac{(s - s_0)^k}{k!} \mathbb{P}_m^{1k} \mathbf{X}_0^{[k+1]} = \sum_{l=0}^{N} \mathbb{P}_m^l \mathbf{X}_0^{[l]} \Big/ \sum_{j=0}^{L} \mathbf{Q}_j^* \mathbf{X}_0^{[j]}.$$

Introducing $\mathbb{C}_m^k = ((s - s_0)/(k-1)!)\,\mathbb{P}_m^{1\,(k-1)}$ one can evaluate

$$\mathbb{C}_m^k = \mathbb{P}_m^k - \sum_{j=0}^{L} \mathbf{Q}_j^* \otimes \mathbb{C}_m^{k-j}, \quad 1 \le k \le N, \tag{7}$$

$$\mathbb{C}_m^k + \sum_{j=1}^{L} \mathbf{Q}_j^* \otimes \mathbb{C}_m^{k-j} = 0, \quad k > N. \tag{8}$$

The knowledge of the series for $\mathcal{M}_m \circ \mathbf{X}_0$, and vector coefficients of the denominator $\mathbf{Q}_j$ allows us to determine (N, L)-approximant for $\mathcal{M}_m \circ \mathbf{X}_0$ from the L first equations (8). The matrix coefficients of the numerator $\mathbb{P}_m^k$ are determined from eq. (7) for $0 \le k \le N$. The linear algebraic system (8) of the L-th order can be called a generalized Hankel system.

Let us consider two examples for $n = 2$.

Example 1. Let be $m = 2$, i.e. we have the following equations (in this case the corresponding hamiltonian has the form $\mathcal{H}_3 = bx^3 + ax^2 P_x$)

$$\frac{dx}{dt} = ax^2, \quad \frac{dP_x}{dt} = bx^2 - 2axP_x,$$

where the right side eq. (1) can be written as $\mathbf{F}_2 = \mathbb{F}_2\mathbf{X}^{[2]}$ with the matrix

$$\mathbb{F}_2 = \begin{pmatrix} a & 0 & 0 \\ b & -2a & 0 \end{pmatrix}.$$

Let be $L = 1$, then expression for $\mathbf{Q}_1$ degenerates into a single equation

$$\mathbb{C}_2^{N+1} = -\mathbf{Q}_1^* \otimes \mathbb{C}_2^N,\ \text{where}\ \mathbb{C}_2^{k+1} = \frac{(s - s_0)^k}{k!} \mathbb{P}_2^{1k}.$$

Equations for matrix coefficients of the numerator $\mathbb{P}_2^k$, $k \ge 1$ can be also reduced:

$$\mathbb{P}_2^k = \mathbb{C}_2^k + \mathbf{Q}_1^* \otimes \mathbb{C}_2^{k-1}, \quad k \ge 1.$$

With regard to the expressions for $\mathbb{P}_2^{1k}$, one can write the following recurrent formula for $\mathbb{C}_2^k$:

$$\mathbb{C}_2^k = \frac{1}{k-1} \mathbb{C}_2^{k-1} \mathbb{G}_2^{\oplus(k-1)}.$$

For guaranteeing required accuracy of the presentation one has to put the following condition:

$$\mathbb{C}_2^{N+1} + \mathbf{Q}_1^* \otimes \mathbb{C}_2^N = 0.$$

The expressions for matrices $\mathbb{P}_2^k$ ($k = \overline{1,4}$) can be obtained using direct evaluations:

$$\mathbb{P}_2^0 = 0,\ \mathbb{P}_2^1 = \mathbb{E},\ \mathbb{P}_2^2 = \mathbb{G}_2 + \mathbf{Q}_1^* \otimes \mathbb{E},$$

$\mathbb{P}_2^3 = \dfrac{1}{2}\mathbb{C}_2^2\mathbb{G}_2^{\oplus 2} + \mathbf{Q}_1^* \otimes \mathbb{C}_2^2,\ \mathbb{P}_2^4 = \dfrac{1}{3}\mathbb{C}_m^3\mathbb{G}_2^{\oplus 3} + \mathbf{Q}_1^* \otimes \mathbb{C}_2^3, \dots$
The final solution can be written in the following form

$$\mathbf{X} = \frac{\mathbf{X}_0 + \mathbb{P}_2^2\mathbf{X}_0^{[2]} + \mathbb{P}_2^3\mathbf{X}_0^{[3]} + \mathbb{P}_2^4\mathbf{X}_0^{[4]}}{1 + \mathbf{Q}_1^*\mathbf{X}_0}.$$

We should note that sequence breaking for $\mathbb{P}_2^k$ may be not take place. In this case instead of polynomial $\mathbf{P}_N(\mathbf{X})$ one obtains a series for some entire function $\mathbf{P}_\infty(\mathbf{X})$ (see an example 2).

It is not difficult to make sure that we can easily to evaluate solution for inverse order of phase vector components with the help of a permutation matrix $\mathbb{U}$, reversing the order of phase vector components $\tilde{\mathbf{X}} = \mathbb{U}\mathbf{X}$: $\tilde{\mathbf{F}}_m(\mathbf{X}) = \mathbf{F}_m(\tilde{\mathbf{X}}) = \mathbb{U}\mathbb{F}_m\mathbb{U}^{-[m]}\tilde{\mathbf{X}}^{[m]} = \tilde{\mathbb{F}}_m\tilde{\mathbf{X}}^{[m]}$. In our case it is corresponds to transfer from hamiltonian $\mathcal{H}_3 = bx^3 + ax^2P_x$ to hamiltonian $\tilde{\mathcal{H}}_3 = axP_x^2 + bP_x^3$.

Example 2. The similar computations can be produced for the case $m = 3$, i.e. for the function $\mathbf{F}_3 = \mathbb{F}_3\mathbf{X}^{[3]}$ with the matrix

$$\mathbb{F}_3 = \begin{pmatrix} 0 & -4a & 0 & 0 \\ 0 & 0 & 4a & 0 \end{pmatrix} = 4a\begin{pmatrix} \mathbb{O}_1 & \mathbb{I} & \mathbb{O}_1 \end{pmatrix},$$

where $\mathbb{O}_k$ is a matrix $2 \times k$ with zero elements, $\mathbb{I} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$. The corresponding hamiltonian is equal to $\mathcal{H}_4 = 2ax^2P_x^2$. For $\mathbb{F}_3$ we have $L = 0$, and denominator is reduced to 1. It should be noted that, as we have $m = 3$, then $k(m-1)+1 = 2k+1$, and therefore the required expression contains only odd degrees of $\mathbf{X}$. After some evaluations one can write

$$\mathbb{P}_3^{2k} = \mathbb{O},\ \mathbb{P}_3^1 = \mathbb{E},\ \mathbb{P}_3^{2k+1} = \frac{(4a(s-s_0))^k}{k!}\mathbb{Q}_k, \quad (9)$$

$$\mathbb{Q}_k = \begin{pmatrix} \mathbb{O}_k & \mathbb{I}^k & \mathbb{O}_k \end{pmatrix},\ \mathbb{I} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (10)$$

From eqs. (9), (10) there follows the required result

$$\exp\mathcal{L}_{\mathbf{F}_3}\circ\mathbf{X} = \exp\left\{4a(s-s_0)\mathbb{I}\mathbf{E}_2^*\mathbf{X}^{[2]}\right\}\mathbf{X},\ \mathbf{E}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}.$$

All similar evaluations can be produced in a symbolic form (using computer algebra codes, i.e. Maple or Mathematica) for some types of homogeneous functions $\mathbf{F}_k(\mathbf{X})$. It is not difficult to see that analogous computations can be produced for other types of rather simple functions $\mathbf{F}_k(\mathbf{X})$ or hamiltonians $\mathcal{H}_k(\mathbf{X})$.

Multiplication Decomposition for a Propagator

All existing multiplication decompositions are based on the well known CBH-formula. The differences between them consists in various forms of a Lie map presentation. One of the most popular and effective example of decomposition is the well known Dragt–Finn factorization, presenting an infinite product of exponential maps, associated with homogeneous polynomials [12]. Some other cases there use an information on corresponding Lie algebra structure, i.e. Lie algebra generators. For finite-dimensional algebras one can obtain results in the form of finite products, otherwise he has to truncate this product with some accuracy using only M terms. Here it can be mentioned factorization schemes, based on approximating decomposition (see, i.e. [3, 13]). All these representation can be used for search of homogeneous forms of polynomials. In the present work we use a combination of existing approaches for searching of the propagator decomposition, satisfied to the Condition 1. Corresponding computations can be done in a symbolic form (using, for example, another approaches, see i.e. [14]).

CONCLUSION

The described procedure of searching exact representation for beam propagator (generated by homogeneous polynomials $\mathbf{F}_m(\mathbf{X}) = \mathbb{F}_m\mathbf{X}^{[m]}$ $(m \geq 2)$ is reduced to algebraic manipulation on matrices $\mathbb{F}_m$ (compare with [15]). These representations are symplectic. The decomposition procedure allows to present required solutions in the form (3). Resulting approximating propagator will be symplectic as expected.

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