APPLICATION OF A NEW CLASS OF SYMPLECTIC INTEGRATORS TO ACCELERATOR TRACKING *

L. Nadolski† and J. Laskar, IMCCE–CNRS, Paris, France

Abstract

The dynamics of particle accelerator beams is commonly described by a Hamiltonian of the form $\mathcal{H} = A + \epsilon B$ where A and B are integrable. Using Lie formalism, we give an overview of a new class of symplectic integrator [1] particularly well adapted when ϵB is viewed as a perturbation of A. These integrators with positive step size can be constructed with a remainder of arbitrary order n in A and order 2 in ϵB. Moreover a corrector step can be added to the integration scheme in many cases such that the remainder becomes actually of order 4 in ϵB. A comparison with the fourth-order standard Forest and Ruth integrator [2] is performed showing in general one order of magnitude improvement in computation precision for the same cost. The construction of these integrators is given for the main magnetic elements of an electron storage ring.

1 SYMPLECTIC INTEGRATION

1.1 Introduction

Symplectic integrators are powerful tools now implemented in most of the tracking codes in accelerator physics. The property of area conservation is particularly suitable for integrating the equations of particle motion over thousands of turns for lepton machines and millions of turns for hadron accelerators. Throughout this article we focus on explicit integration methods. For a large enough ring, the dynamics of the particle is modelled by representing each magnet by a separate Hamiltonian. Its ¤ow $\mathcal{M}$ can be computed, *i.e.* the map linking the particle coordinates at the entrance, $\vec{X}^i$ and the exit, $\vec{X}^f$. The ¤ow of the full ring is then obtained by concatenating the ¤ows of each single element of the ring.

1.2 Magnet model

In general the dynamics of a particle through one magnetic element is well described by an autonomous Hamiltonian of the form $\mathcal{H} = A + \epsilon B$, where A and B are both integrable. Moreover ϵB can often be seen as a perturbation of A (but this is not necessarily always true). For a particle whose positions q_j are denoted (x, y, l) and canonical conjugate momenta p_j denoted (p_x, p_y, δ), the equations of motion are given by:

$$\frac{d\vec{X}}{ds} = \{\mathcal{H}, \vec{X}\} = L_{\mathcal{H}}\vec{X}, \qquad (1)$$

where $\vec{X}$ is the full coordinate vector and $L_{\mathcal{H}}$ the Lie derivative operator de£ned by $L_{\mathcal{H}} f = \sum_{j=1}^{3} \frac{\partial \mathcal{H}}{\partial p_j}\frac{\partial f}{\partial q_j} - \frac{\partial \mathcal{H}}{\partial q_j}\frac{\partial f}{\partial p_j}$. Formally the solution of Eq. 1 is:

$$\vec{X}^f = \sum_{n\geq 0} \frac{s^n}{n!} L_{\mathcal{H}}^n \vec{X}^i = e^{sL_{\mathcal{H}}}\vec{X}^i. \qquad (2)$$

1.3 Construction principle

Explicit symplectic integrators are obtained by approximating the exponential $e^{sL_{\mathcal{H}}} = e^{s(L_A + L_{\epsilon B})}$ by products of the integrable ¤ows e^{csL_A} and $e^{dsL_{\epsilon B}}$. L_A and $L_{\epsilon B}$ usually do not commute, but the well known Backer–Campbell–Hausdorff theorem states that

$$e^{sL_A} e^{sL_{\epsilon B}} = e^{sL_{\tilde{\mathcal{H}}}}, \qquad (3)$$

where $\tilde{\mathcal{H}}$ is the formal Hamiltonian:

$$\tilde{\mathcal{H}} = A + \epsilon B + \frac{s}{2}\{A, \epsilon B\} + \frac{s^2}{12}\left(\{A\{A, \epsilon B\}\} + \{\epsilon B\{\epsilon B, A\}\}\right) + \dots \qquad (4)$$

Then nth-order integrators $S_n(s)$ can be constructed:

$$e^{sL_{\tilde{\mathcal{H}}}} = \prod_{i=1}^{n} e^{c_i s L_A} e^{d_i s L_{\epsilon B}} + \mathcal{O}(s^n\epsilon) = S_n(s) + \mathcal{O}(s^n\epsilon), \qquad (5)$$

where the coef£cients $(c_i, d_i)_{i=1..n}$ are determined to get a remainder of order n. By choosing a class of symmetric integrator, *i.e.* $S_n^{-1}(s) = S_n(-s)$, Equation 4 leads to a remainder of even order. The simplest integrator of this kind is the leapfrog integrator introduced by Ruth [3]

$$S_2(s) = e^{c_1 s L_A} e^{d_1 s L_{\epsilon B}} e^{c_1 s L_A}, \qquad (6)$$

with $c_1 = \frac{1}{2}$ and $d_1 = 1$. The usual 4th-order Forest and Ruth integrator [2] is,

$$S_4(s) = e^{d_1 s L_A} e^{c_2 s L_{\epsilon B}} e^{d_2 s L_A} e^{c_3 s L_{\epsilon B}} e^{d_2 s L_A} e^{c_2 s L_{\epsilon B}} e^{d_1 s L_A} \qquad (7)$$

with $c_2 = \frac{1}{1+\alpha}$, $c_3 = (\alpha - 1)c_2$, $d_1 = \frac{c_2}{2}$, $d_2 = \alpha d_1$, and $\alpha = 1 - 2^{\frac{1}{3}}$.

2 NEW CLASS OF SYMPLECTIC INTEGRATORS

2.1 De£nitions

The integrators we deal with in this section are described in detail in reference [1]. They can be divided into two general classes $\mathcal{SABA}_k$ and $\mathcal{SBAB}_k$:

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† LBNL, Berkeley, CA 94720, USA; lsnadolski@lbl.gov.

$$\begin{aligned}
\mathcal{SABA}_{2n} \;&: e^{c_1 s L_A} e^{d_1 s L_{\epsilon B}} \dots e^{d_n s L_{\epsilon B}} \\
&\quad e^{c_{n+1} s L_A} e^{d_n s L_{\epsilon B}} \dots e^{d_1 s L_{\epsilon B}} e^{c_1 s L_A} \\
\mathcal{SABA}_{2n+1} \;&: e^{c_1 s L_A} e^{d_1 s L_{\epsilon B}} \dots e^{c_{n+1} s L_A} e^{d_{n+1} s L_{\epsilon B}} \\
&\quad e^{c_{n+1} s L_A} \dots e^{d_1 s L_{\epsilon B}} e^{c_1 s L_A} \\
\mathcal{SBAB}_{2n} \;&: e^{d_1 s L_{\epsilon B}} e^{c_2 s L_A} e^{d_2 s L_{\epsilon B}} \dots e^{d_n s L_{\epsilon B}} \\
&\quad e^{c_{n+1} s L_A} e^{d_n s L_{\epsilon B}} \dots e^{d_2 s L_{\epsilon B}} e^{c_2 s L_A} e^{d_1 s L_{\epsilon B}} \\
\mathcal{SBAB}_{2n+1} \;&: e^{d_1 s L_{\epsilon B}} e^{c_2 s L_A} e^{d_2 s L_{\epsilon B}} \dots e^{c_{n+1} s L_A} \\
&\quad e^{d_{n+1} s L_{\epsilon B}} e^{c_{n+1} s L_A} \dots e^{d_2 s L_{\epsilon B}} e^{c_2 s L_A} e^{d_1 s L_{\epsilon B}}
\end{aligned} \tag{8}$$

For instance, the second order leapfrog integrator belongs to $\mathcal{SABA}_1$ with the formal Hamiltonian is $\tilde{\mathcal{H}} = A + \epsilon B + \mathcal{O}(s^2\epsilon)$. The Forest–Ruth integrator belongs to $\mathcal{SABA}_3$ with $\tilde{\mathcal{H}} = A + \epsilon B + \mathcal{O}(s^4\epsilon)$. For this integrator two steps are negative, which implies the absolute value of some steps to be quite large for a total unity step size: $d_1 \approx 0.6756$, $d_2 \approx \mathbf{-0.1756}$, $c_2 \approx 1.3512$, and $c_3 \approx \mathbf{-1.7024}$. As a result, for large integration step sizes the method is less ef£cient (ef£ciency, numerical instability). In fact, Suzuki proved the impossibility to construct an integrator of order $n \geq 3$ with only positive step sizes [4].

2.2 Improvement

The negative step size problem can be partially solved. In the previous section the existence of the small parameter ϵ has not been taken into account. The method consists in determining the coef£cients (c_j, d_j) for the integrators (8) in order to get a remainder of order $\mathcal{O}(s^n\epsilon + s^2\epsilon^2)$ (versus $\mathcal{O}(s^n\epsilon)$). For an integrator of the class $\mathcal{SABA}_2$, one gets

$$SABA_2 = e^{c_1 s L_A} e^{d_1 s L_{\epsilon B}} e^{c_2 s L_A} e^{d_1 s L_{\epsilon B}} e^{c_1 s L_A}, \tag{9}$$

with a unique solution for the coef£cients $d_1 = \frac{1}{2}$, $c_1 = \frac{1}{2}(1 - c_2)$, and $c_2 = \frac{1}{\sqrt{3}}$ with

$$\tilde{\mathcal{H}} = A + \epsilon B + \underbrace{s^2\epsilon^2\left(-\frac{1}{24} + \frac{c_1}{4}\right)\{\{A,B\},B\} + \mathcal{O}(s^4\epsilon)}_{\mathcal{O}(s^4\epsilon + s^2\epsilon^2)}. \tag{10}$$

Similarly for the class $\mathcal{SBAB}_2$,

$$SBAB_2 = e^{d_1 s L_{\epsilon B}} e^{c_2 s L_A} e^{d_2 s L_{\epsilon B}} e^{c_2 s L_A} e^{d_1 s L_{\epsilon B}}, \tag{11}$$

with the unique triplet $d_1 = \frac{1}{6}$, $d_2 = \frac{2}{3}$, and $c_2 = \frac{1}{2}$.

Actually, in the particular case where A is quadratic in the momenta and B depends only on the positions, the method can be improved by introducing a corrector $\mathcal{C}$ de£ned by (see Ref. [1]):

$$\mathcal{C} = e^{-s^3\epsilon^2 \frac{c}{2} L_{\{\{A,B\},B\}}}, \tag{12}$$

where the c coef£cient is obtained by zeroing the term of order $\mathcal{O}(s^2\epsilon^2)$ (see for instance the Eq. 10 for the integrator $SABA_2$). We should emphasize that the corrector step size is negative. Nevertheless the higher order the integrator is the smaller corrector step size is (see Tab. 1).

n	$SABA_n$	$SBAB_n$
1	$1/12$	$-1/24$
2	$(2-\sqrt{3})/24$	$1/72$

Table 1: Coef£cient for the corrector (from Ref. [1]).

So a full integrator scheme becomes (*e.g.* for $SABA_2$):

$$SABAC_2 = \mathcal{C}\,(SABA_2)\,\mathcal{C} \tag{13}$$

This second order integrator is symmetric and of remainder of order $\mathcal{O}(s^n\epsilon + s^4\epsilon^2)$.

3 SIMULATION AND APPLICATION

3.1 Single element integration

The previously explained scheme of integration was applied to write a modular tracking code in Fortran90. As illustration the symplectic applications for a straight section, a combined dipole and a sextupole are given.

Straight section The Hamiltonian of a straight section for an ultra relativistic particle can be written as:

$$\mathcal{H}(x,y,l,p_x,p_y,\delta) = \frac{p_x^2 + p_y^2}{2(1+\delta)}. \tag{14}$$

The integration of the equations of motion is then trivial:

$$\begin{cases} x^f &= x^i + \frac{p_x^i}{1+\delta}s \\ y^f &= y^i + \frac{p_y^i}{1+\delta}s \\ l^f &= l^i - \frac{(p_x^i)^2+(p_y^i)^2}{2(1+\delta)^2}s \end{cases} \qquad \begin{cases} p_x^f &= p_x^i \\ p_y^f &= p_y^i \\ \delta^f &= \delta \end{cases} \tag{15}$$

Combined dipole The Hamiltonian of a combined dipole can be written in the approximation of large rings,

$$\mathcal{H} = \underbrace{\frac{p_x^2 + p_y^2}{2(1+\delta)}}_{A(p_x,p_y,\delta)} \underbrace{-h\delta x + h^2\frac{x^2}{2} + \frac{b_2}{2}(x^2 - y^2)}_{B(x,y,l)}, \tag{16}$$

where h and b_2 are the curvature and the quadrupole focusing of the magnet. Whatever the integrator to be used ($\mathcal{SABA}_n$ or $\mathcal{SBAB}_n$) only the two operators e^{sL_A} and e^{sL_B} have to be calculated. For A and B, the results are:

$$e^{sL_A} : \begin{cases} x^f = & x^i + \frac{p_x^i}{1+\delta}s \\ y^f = & y^i + \frac{p_y^i}{1+\delta}s \\ l^f = & l^i - \frac{(p_x^i)^2+(p_y^i)^2}{2(1+\delta)^2}s \\ & -hx^i s - h\frac{p_x^i}{1+\delta}\frac{s^2}{2} \end{cases} \qquad \begin{cases} p_x^f &= p_x^i \\ p_y^f &= p_y^i \\ \delta^f &= \delta \end{cases} \tag{17}$$

$$e^{sL_B} : \begin{cases} x^f &= x^i \\ y^f &= y^i \\ l^f &= l^i \end{cases} \qquad \begin{cases} p_x^f &= p_x^i - \left((b_2 + h^2)x^i - h\delta\right)s \\ p_y^f &= p_y^i + b_2 y^i s \\ \delta^f &= \delta \end{cases} \tag{18}$$

This integrator can be improved by computing the following double Poisson bracket as stated previously:

$$C = \{\{A, B\}, B\} = \frac{1}{1+\delta}\left((kx-\delta h)^2 + b_2^2 y^2\right), \quad (19)$$

with $k = b_2 + h^2$. The corrector scheme is then:

$$e^{sL_C} : \begin{cases} x^f &= x^i \\ y^f &= y^i \end{cases} \quad \begin{cases} p_x^f &= p_x^i - \frac{2k(kx^i - \delta h)}{1+\delta} s \\ p_y^f &= p_y^i - \frac{2b_2^2}{1+\delta} y^i s \end{cases} \quad (20)$$

with $s = -s^3 \frac{c}{2}$. This result can be directly used for a pure quadrupole magnet by choosing $h = 0$.

Sextupole The Hamiltonian of a normal sextupole of strength S is:

$$\mathcal{H} = \underbrace{\frac{p_x^2 + p_y^2}{2(1+\delta)}}_{A(p_x, p_y, \delta)} + \underbrace{\frac{S}{3}(x^3 - 3xy^2)}_{B(x,y,l)}. \quad (21)$$

The A part is just the Hamiltonian of a straight section (see Eq. 15). The symplectic map for B is simply:

$$e^{sL_B} x^i : \begin{cases} x^f &= x^i \\ y^f &= y^i \\ l^f &= l^i \end{cases} \quad \begin{cases} p_x^f &= p_x^i - S(x^2 - y^2)\, s \\ p_y^f &= p_y^i + 2Sxy\, s \\ \delta^f &= \delta \end{cases} \quad (22)$$

3.2 Comparison with Forest-Ruth scheme

The accuracy of this new class of integrators has been studied systematically for the main elements of a storage ring. Figure 1 shows an application for a combined magnet (dipole and quadrupole) whose Hamiltonian is given by Eq. 16 and with $h = 0.2015$ m^{-1}, $b_2 = -4 \times 10^{-3}$ m^{-2}, and a length $L = 0.86$ m.

The relative error of the energy conservation is plotted with respect to the integration step size at constant number of evaluations of exponential terms using a log–log scale over one thousand turns through the magnet. All three integrators are of order 4. The integrator $SABA_2$ implemented with its corrector is the most precise with a precision one order of magnitude higher than the Forest and Ruth integrator. Practically this means that for a given accuracy these new integrators are faster, in average one step of integration can be saved for each magnet.

Another quality of this class of integrators is its better numerical stability. This is a direct result of the integrator coef£cients. This is graphically shown in Fig. 2. The integration step sizes are small and much smaller on the entrance and exit faces of the magnet.

4 CONCLUSION

This new class of integrators proves to be better than the traditional fourth-order Ruth integrator. They are used in a new tracking code to model current storage rings such as the ALS, Super-ACO, and SOLEIL. This code includes also small machine effects and quadrupole fringe £elds. A direct application is given in the reference [5].

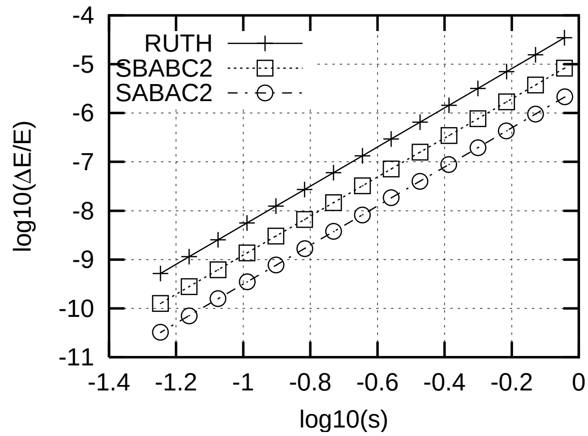

Figure 1: Relative energy error versus integration step size in logarithmic scale. The integrators $SABA_2$ and $SBAB_2$ with correctors are more precise than the Forest and Ruth S_4 integrator by respectively one order and half a order of magnitude at the same cost.

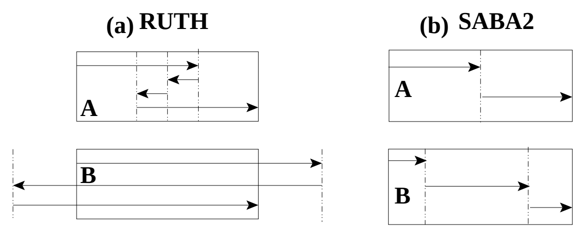

Figure 2: Integration scheme of A and B for the Forest and Ruth integrator S_4 (a) and $SABA_2$ integrator (b).

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