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A BENCHMARK STUDY OF A HIGH ORDER SYMPLECTIC INTEGRATION METHOD WITH ONLY POSITIVE STEPS

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Abstract

The symplectic integrators CSABA & CSBAB are used in order to calculate single particles dynamics in accelerators and storage rings. These integrators include only forward drift steps while being highly accurate. Their efficiency to describe various optical and dynamical quantities for main magnetic elements and non-linear lattices is calculated and compared with the efficiency of the splitting methods used in MAD-X - PTC.

INTRODUCTION

The good understanding of a non-linear system relies on the accurate knowledge of the evolution of the dynamic variables, for a great interval of the independent variable ("time"). In particular in an accelerator, the machine performance can be understood by studying the particles' motion for a large number of turns. The tracking studies are performed with particle simulators, which are fast and accurate enough. These attributes of a tracking program, including the preservation of the Hamiltonian structure of the system, can be obtained if a symplectic integration scheme is used.

A perturbed Hamiltonian written in the usual form $\mathcal{H} = A + \epsilon B$ can describe the particles' motion in an accelerator. For such Hamiltonians, where both A and B are independently integrable, a new set of symmetric symplectic integrators was proposed by McLachlan [1]. Later, in a more generalized work by Laskar and Robutel [2], the CSABA$_\nu$ & CSBAB$_\nu$ symplectic integrators were introduced. Although it was shown that generic symplectic integration schemes of order $\zeta > 2$ have to include by construction negative "time" steps [3], these particular integrators and for the Hamiltonians that we are interested in (certain forms of A and B), have only forward steps. In this paper, the performance of these integrators is compared against other well established ones, namely the famous Yoshida, Forest and Ruth (YFR$_\nu$) integrators [4–6] and the improved TEAPOT$_\nu$ ones [7] that are used in MAD-X - PTC [8].

CSABA$_\nu$ & CSBAB$_\nu$ INTEGRATORS

For this work, the Lie algebra is used and its multiplication rule is defined by the Poisson brackets $\omega \bullet \upsilon = \{\omega(q,p), \upsilon(q,p)\} = \sum_{j=1}^{N} \left[\frac{d\omega}{dp_j}\frac{d\upsilon}{dq_j} - \frac{d\omega}{dq_j}\frac{d\upsilon}{dp_j} \right]$. In this framework, any symplectic map can be described by one or more Lie transformations e^{L_K} where L_K is the Lie operator which is defined by $L_\omega \upsilon = \{\omega, \upsilon\}$. The map $\mathcal{M}$ that describes the Hamiltonian flow from the initial position s_i to a final one s_f is shown in the following formal solution:

$$\vec{\mathbf{X}}_\mathbf{f} = \mathcal{M}\,\vec{\mathbf{X}}_\mathbf{i} = \sum_{n\geq 0} \frac{\lambda^n}{n!} L^n_{\mathcal{H}}\,\vec{\mathbf{X}}_\mathbf{i} = e^{\lambda\, L_{\mathcal{H}}}\vec{\mathbf{X}}_\mathbf{i}\,, \qquad (1)$$

with $\lambda = s_f - s_i$. The vector $\vec{\mathbf{X}}(s_i) \equiv \vec{\mathbf{X}}_\mathbf{i}$ consists of the initial conditions of the conjugate dynamic variables $\vec{\mathbf{X}} = (q_1, p_1, \ldots, q_N, p_N)$.

A problem that is not integrable by making use of the classical form of the Hamilton's equations, is also not solvable if the Eq. (1) is used. It should be mentioned that any truncation of the summation in Eq. (1) will break the symplecticity of the solution. The significance of Eq. (1) becomes clear when the Backer-Campbell-Hausdorff (BCH) theorem is used. According to this and if A and B do not commute ($\{A, B\} \neq 0$), any Lie transformation $e^{\lambda\, L_{\mathcal{H}}} = e^{\lambda(L_A + L_{\epsilon B})}$ is equally expressed by an infinite concatenation of the Lie transformations $e^{c_j\,\lambda\, L_A}$ and $e^{d_j\,\lambda\, L_{\epsilon B}}$, $e^{\lambda\, L_{\mathcal{H}}} = e^{\lambda(L_A+L_{\epsilon B})} = \prod_{j=1}^{\infty} e^{c_j\,\lambda\, L_A}\, e^{d_j\,\lambda\, L_{\epsilon B}}$. Keeping terms up to $j = \mathcal{N}$ and choosing appropriately the values of c_j and d_j, for A and B being independently integrable, a symplectic integrator of order ζ ($O(\lambda^\zeta)$) for the Hamiltonian $\mathcal{H}$ is formed as $\prod_{j=1}^{\mathcal{N}} e^{c_j\,\lambda\, L_A}\, e^{d_j\,\lambda\, L_{\epsilon B}} + O(\lambda^\zeta) = e^{\lambda\, L_{\mathcal{H}}}$. In [1, 2] the procedure for the construction of the SABA$_\nu$ & SBAB$_\nu$ symplectic integrators of order $O(\lambda^{2\nu}\epsilon + \lambda^2\epsilon^2)$ can be found.

The studied Hamiltonian has the general form $H = A(q^n \cdot p^2) + B(q^m)$ with $n = 0, 1$ & $m = 0, 1, 2, \ldots$. The function A describes the contribution of the kinematic terms even in curved trajectory (n=1) and B expresses the contribution from the electromagnetic fields. For such Hamiltonians, the term $\mathcal{F} = \{\{A, B\}, B\}$ is integrable. In this case a the corrector step $e^{-\frac{1}{2}\lambda^3\epsilon^2 f_\nu L_{\mathcal{F}}}$ can be added at the beginning and the end of the SABA$_\nu$ & SBAB$_\nu$ in order to eliminate the $\lambda^2\epsilon^2$ dependence of the remainder. The resulted CSABA$_\nu$ & CSBAB$_\nu$ integrators [2] are of order $O(\lambda^{2\nu}\epsilon + \lambda^4\epsilon^2)$. The general form of $\mathcal{F}$ for different multipoles, except for dipoles ($m = 1$), is a non-Maxwellian potential given by:

$$\mathcal{F}(x, y) = \frac{1}{1+\delta}\left(\frac{eB_0}{P_0}h_m\right)^2 r^{2(m-1)}\,. \qquad (2)$$

$h_m \equiv (b_m, a_m)$ is the $(2m)^{th}$ multipole coefficient, with b_m refers to the normal and a_m to the skew multipole. B_0 is the main dipole field, P_0 is the reference momentum, e is the electric charge, $r = \sqrt{x^2 + y^2}$ and δ is the relative energy deviation.

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BENCHMARKING STUDIES

In order to compare the performance of the CSABA$_\nu$ & CSBAB$_\nu$ against TEAPOT$_\nu$ [7] and YFR$_\nu$ integrators [5, 6], various analytical and tracking studies are undertaken. For all the linear and non-linear analytical studies, the presented quantities are expressed as a function of the quadrupoles length (LQ) and their normalized strength (KQ).

Analytical Studies - Phase Advance Calculation

The advance in phase μ caused by passing through a linear FODO cell can be calculated from the relation $\cot(\mu) = \frac{M_{1,1}}{M_{1,2}}\beta_i - \alpha_i$. The β_i and α_i are the Courant-Snyder parameters at the beginning of the FODO cell and the $M_{j,k}$ are the elements of the FODO's transfer matrix. Since the optical functions β_i and α_i are the same for any integrator, the relative difference of the ratio $M_{1,1}/M_{1,2}$ from the target value $M^q_{1,1}/M^q_{1,2}$ is studied. The map M^q is the exact map for a quadrupole. In Fig. 1 the results of the CSABA$_2$ (Fig. 1b) and the TEAPOT$_5$ (Fig. 1a) are presented. Being interested in the area enclosed by the white dashed curve, where the stability of the motion is guaranteed, the CSABA$_2$ is more accurate than the TEAPOT$_5$ across the KQ - LQ plane, even if TEAPOT$_5$ consists of more maps, 11 in contrast to 7 of the CSABA$_2$. For some combinations of the KQ & LQ, among which are the ones of the LHC and HL-LHC, the CSABA$_2$ is around one order of magnitude more accurate. Indeed, the CSABA$_\nu$ and the CSBAB$_\nu$ are not only more accurate than TEAPOT but they are also more economical with respect to the integration time.

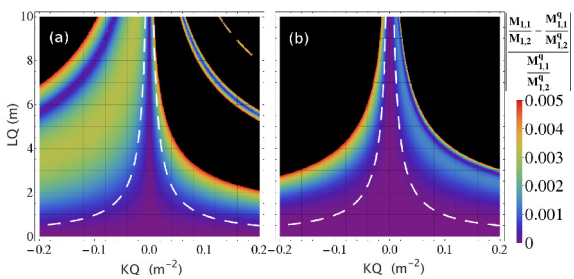
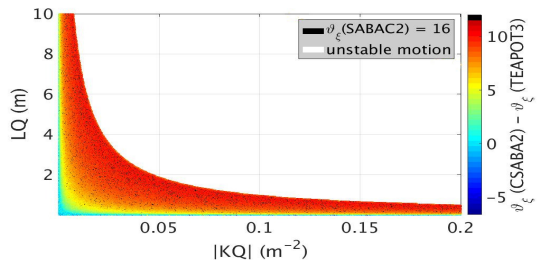


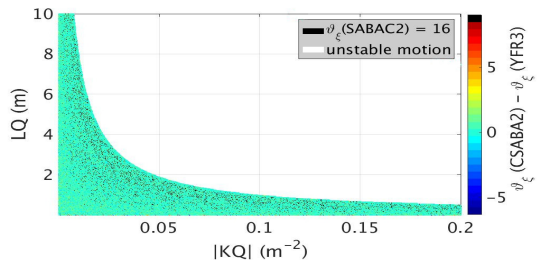
Figure 1: The absolute value of the relative difference of the ratio $M_{1,1}/M_{1,2}$ from the ratio $M^q_{1,1}/M^q_{1,2}$ as a function of different KQ and LQ, for the TEAPOT$_5$ (a) and the CSABA$_2$ (b). The area under the white dashed lines guarantees stable motion through a symmetric FODO cell.

Analytical Studies - Chromaticity & Tune Shift with Amplitude Calculation

Using the integrators CSABA$_2$, TEAPOT$_3$ and YFR$_3$, the chromaticity induced by the sextupoles, noted as ξ, in a non-linear FODO cell with zero horizontal and vertical total chromaticity is calculated. In order to have the same optical functions for all the different studies, the symplectic integrators are only used for the non-linear elements of the lattice. The difference of the accuracy order, for the couples CSABA$_2$ & TEAPOT$_3$ and CSABA$_2$ & YFR$_3$ is shown in Fig. 2. The CSABA$_2$ is the most accurate of the three across the area that guarantees stable motion. Compared to the TEAPOT$_3$ (Fig. 2a) the accuracy difference varies for different KQ & LQ values. For the LHC and HL-LHC parameters the CSABA$_2$ is at least six orders more accurate. Compared to YFR$_3$ (Fig. 2b), the CSABA$_2$ is more accurate by one order for any value of the KQ & LQ. The accuracy degradation of the TEAPOT$_3$, for larger values of KQ & LQ, seems to be an inherent problem of that integrator family. Since they are constructed to reproduce very accurately the $M^q_{2,1}$ element of the quadrupole's transfer matrix, they start loosing in accuracy for higher order multi-pole magnets as compared to a Hamiltonian-centric integrator such as the CSABA$_\nu$ & CSBAB$_\nu$. The black dots in Fig. 2 are points where the CSABA$_2$ is accurate up to the 16^{th} decimal digit of the chromaticity value, i.e. it reaches machine precision.



(a)



(b)

Figure 2: The difference of the accuracy order between CSABA$_2$, TEAPOT$_3$ and YFR$_3$ for the sextupoles chromaticity calculation.

For the same lattice, the tune shift with amplitude is calculated and the results are displayed in Fig. 3. Again the CSABA$_2$ is at least one order more accurate than YFR$_3$. Similar results showing the comparison between the CSABA$_2$ and the YFR$_3$ can be found in [9].

Tracking Studies - Tune diffusion

The above analytical studies are useful indicators for the power of the novel integrators. Nevertheless, only particle tracking provide a detailed understanding of the dynamics. For these studies, a lattice similar to the one of the LHC is used. In order to obtain the target values, an "exact" symplectic integrator is constructed. This integrator is composed by the exact solutions for the linear elements and for the nonlinear ones, it uses a splitting method that consists of

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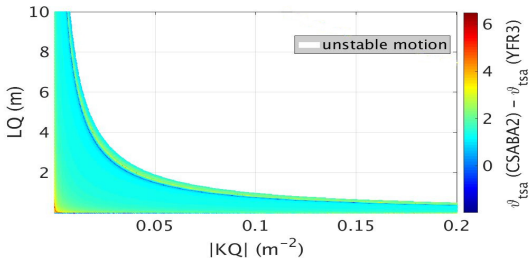

Figure 3: The difference of the accuracy order between $CSABA_2$and YFR_3 for the sextupoles tune shift with amplitude calculation.

5001 drifts which are separated by 5000 kicks. The kicks have the same strength and the drifts the same length.

In Fig. 4, the footprints taken by using the "exact" (yellow) and the $CSABA_2$ (green) integrator are plotted. The agreement of the two footprints is almost perfect.

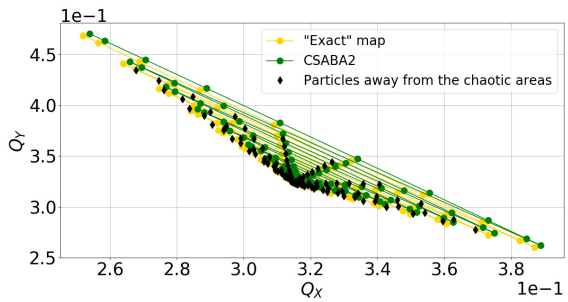

Figure 4: The footprints taken by using the "exact" (yellow) and the $CSABA_2$ (green) integrator can be seen. Particles away from the chaotic areas can be seen are denoted by black rhombus.

The tune of the particles that are not chaotic is invariant. However, the limited accuracy of the integrator that performs the tracking affects the symplecticity and thereby the tunes. The more accurate integrators will be affected less. Using the "exact", the $CSABA_2$ and the $TEAPOT_3$ integrators, the tune diffusion (TD) for particles away from the chaotic areas is calculated (black rhombus in Fig. 4). The tune diffusion is given by the formula $TD = Log_{10}\left(\sqrt{(Q_{X_f} - Q_{X_i})^2 + (Q_{Y_f} - Q_{Y_i})^2}\right)$ where, Q_i is the tune at the first 5000 turns and the Q_f is the tune calculated from the next 5000 turns. For the tune determination, a highly accurate algorithm (NAFF) is used [10–12]. The TDs obtained by using the $CSABA_2$ and the $TEAPOT_3$, are compared with the ones taken by the "exact" integrator (target values). The results can be seen in Fig. 5. In the y-axis the difference of the accuracy order between $CSABA_2$ and $TEAPOT_3$ for the tune diffusion is displayed. With green color are the cases where the $CSABA_2$ is more accurate than the $TEAPOT_3$ and with red the cases that the $TEAPOT_3$ is more accurate. In general, the $CSABA_2$ is superior to the $TEAPOT_3$ since it can capture the right TD for 10 % more particles.

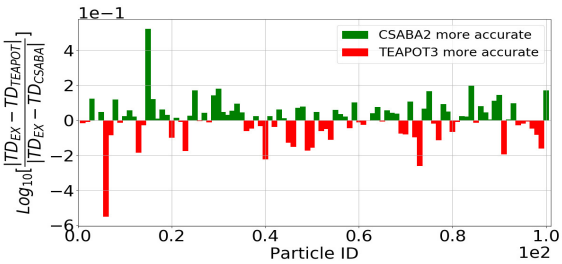

Figure 5: TD accuracy for a set of particles away from th chaotic areas. With green color are the cases where the $CSABA_2$ is more accurate than the $TEAPOT_3$ and with read the cases that the $TEAPOT_3$ is more accurate.

USE OF THE CSABA$_\nu$ & CSBAB$_\nu$ FOR "TIME" DEPENDED POTENTIALS

The symplectic map $\mathcal{M}$ can be calculated from the equation $\dot{\mathcal{M}} = \mathcal{M}L_{\mathcal{H}}$ where the dot over $\mathcal{M}$ indicates derivation with respect to the independent variable (τ). Its solution is given by the following expression:

$$\mathcal{M}(\tau) = exp\left[\int_{\tau_i}^{\tau} L_{\mathcal{H}}\, d\tau'\right] , \qquad (3)$$

if the Poisson bracket $\left\{\mathcal{H}(\vec{\mathbf{X}};\tau_1), \mathcal{H}(\vec{\mathbf{X}};\tau_2)\right\}$ is equal to zero for any two instances of the independent variable τ_1 and τ_2. The last condition is true for every autonomous Hamiltonian. However, any Hamiltonian system with N degrees of freedom and explicit dependence on the independent variable ($\mathcal{H}(\vec{\mathbf{X}}, \tau; \tau)$) can be equally described from a new autonomous Hamiltonian with $N + 1$ degrees of freedom ($\overline{\mathcal{H}}(\vec{\overline{\mathbf{X}}}; \varsigma)$). The new Hamiltonian can be obtained from the generating function $F_2 = \sum_{i=1}^{N} \overline{p}_i q_i + \overline{p}_{N+1}\tau$. Thus, $\overline{\mathcal{H}}(\overline{q}, \overline{p}; \varsigma) = \mathcal{H}(q, p, \tau; \tau) - \mathcal{H}$ by setting $q_i = \overline{q}_i$, $p_i = \overline{p}_i$ for $i = 1, \ldots, N$, $\tau = \overline{q}_{N+1}$ and adding $\overline{p}_{N+1} = -\mathcal{H}$. For any non-autonomous Hamiltonian at which the previous transformation is performed, Eq. (3) can be used, in particular to integrate a 3D field [13]. In order to have only positive steps for the new Hamiltonian $\overline{\mathcal{H}}$, a convenient splitting is described by, $\overline{A}(\overline{q}^n \cdot \overline{p}^2, \overline{p}^n \cdot \overline{q}^m, -\mathcal{H})$ and $\overline{B}(\overline{q}^m, \tau)$ with $n = 0, 1$ and $m = 0, 1, 2, \ldots$. For this splitting, the quantity $\{\{\overline{A}, \overline{B}\}, \overline{B}\}$ is integrable (dependent only on the coordinates) and so, the CSABA$_\nu$ & CSBAB$_\nu$ can be employed.

CONCLUSION

In this paper the new set of symplectic integrators which consists of only forward steps, CSABA$_\nu$ & CSBAB$_\nu$, is compared with the TEAPOT integrators used in MAD-X and Yoshida's 4th order integrator. For all these studies, the CSABA$_\nu$ & CSBAB$_\nu$ are significantly more accurate than the others. These findings indicate that the implementation of these integrators in tracking programs used by the accelerator community (as it is foreseen for the new generation MAD (MAD-NG)) will be very beneficial.

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