COMPARISON OF MATRIX FORMALISM AND STEP-BY-STEP INTEGRATION FOR THE LONG-TERM DYNAMICS SIMULATION IN ELECTROSTATIC FIELDS*

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Abstract

An approach based on matrix formalism for solving differential equations is described. Effective in sense of performance matrix formalism can be tested with less efficient, but accurate traditional algorithm of numerical simulation based on the Runge-Kutta scheme. In both cases the symplectic version of the algorithms are used. The results coincide to analytical calculations, but some disagreements have been identified. The approach implementation is demonstrated in the problem of long-term spin dynamics in electrostatic fields.

INTRODUCTION

Particles dynamics in electromagnetic fields is described by Newton-Lorentz equation. This system of ordinary differential equations can be solve by appropriate numerical methods. In this research two approaches are developed. Firstly, for step-by-step integration a symplectic Runge-Kutta scheme is used. As second approach a mapping algorithm based on matrix formalism [1] is implemented.

In the EDM search COSY Infinity [2] is also used. COSY Infinity is known as a very powerful instrument for particle tracking in electromagnetic fields. The key idea of this research is to develop another high-performnce approach for simulation of spin-orbital dynamics. Both Matrix Formalism and COSY Infinity allow to simulate spin-orbital motion of millions of particles. So these methods can be verified by each other. At present, in the EDM search the MPI (Message Passing Interface) version of the COSY Infinity program is installed on a supercomputer with 310^5 processors. For matrix formalism code we can use OpenMP or OpenCL for running tasks on clasters in St.Petersburg State University (e.g. GPU accelerators).

Due to the fact that one of the tasks in JEDI is examination of spin dynamics in electrostatic fields [3], in this paper magnetic fields are not considered. But all described techniques can be used in common case of electromagnetic fields without modifications.

In the article particle dynamics is considered in 9-dimensional space. A state of dynamic system is described as $(x,\, x',\, y,\, y',\, S_x,\, S_y,\, S_s,\, dv,\, t)$ vector, where x, x' and y, y' are transverse and vertical displacement and velocity respectively; S_x, S_y, S_s are components of spin vector in curvilinear coordinate system (see Fig. 1); $dv = \Delta v/v_0$ is deviation of the initial particle velocity; t is time variable. Note, that a state vector depends on arc length s, which is chosen as an independent variable.

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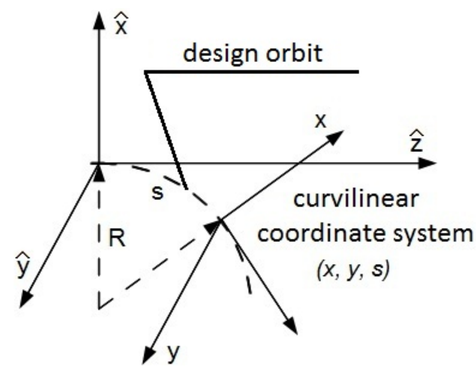

Figure 1: Curvilinear coordinate system.

The mathematical models that used for description of partical motion and spin dynamics are presented in [4]. In this article only numerical approaches are considered.

STEP-BY-STEP INTEGRATION

The Newton-Loretz (particle motion) and BMT (spin dynamics) equations can be written as following system

$$\begin{aligned} \frac{d}{ds}X &= F(s, X), \\ \frac{d}{ds}v_0 &= 0, \end{aligned} \tag{1}$$

where $X = (x, x', y, y', S_x, S_y, S_s, dv, t)$.

This allows us to use classical step-by-step integration methods to solve this system. Article [5] provide both symplectic Runge-Kutta integration schemes, and the algorithm for it derivation up to the 12 order. For the current research a symplectic 2-stage Runge-Kutta scheme of 4 order was implemented.

Table 1: 2-stage 4-order implicit Runge-Kutta scheme

$b_1 + \tilde{c_1}$	$b_1/2$	$b_1/2 + \tilde{c_1}$
$b_1 - \tilde{c_1}$	$b_1/2 - \tilde{c_1}$	$b_1/2$

$$b_1 = 1/2,\ 2b_1\tilde{c_1}^2 = 1/12$$

According to this scheme (Table 1), the solution of the equations (1) can be presented in iterative form

$$\begin{aligned} \mathbf{X}_{n+1} &= \mathbf{X}_n + h\sum_{j=1}^2 b_j \mathbf{F}(s + hc_j, \mathbf{X}^{(i)}), \\ \mathbf{X}^{(i)} &= \mathbf{X}_n + h\sum_{j=1}^2 a_{ij} \mathbf{F}(s + hc_j, \mathbf{X}^{(i)}). \end{aligned}$$

This integration method provide a symplectic solution by choosing of the corredponded coefficients a_{ij}, b_j, c_j.

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MATRIX FORMALISM

As mapping approach matrix formalism is used. It allows to present the solution as set of numerical matrices and operations of multiplication and addition only.

Matrix form of ODE

Under the assumptions of $F(0, X_0) = 0$ the system (1) can be presented in the following form [6]

$$\frac{d}{dt}X = \sum_{k=0}^{\infty} P^{1k}(t)X^{[k]}, \qquad (2)$$

where $X^{[k]}$ is kronecker power of vector X, matrices P^{1k} can be calculate as

$$P^{1k}(t) = \frac{1}{(k)!}\frac{\partial^k F(t, X_0)}{\partial(X^{[k]})^T}, \quad k = 1, 2, \dots$$

Solution of system (2) can be written in form

$$X = \sum_{k=0}^{\infty} R^{1k}(t)X_0^{[k]}. \qquad (3)$$

Elements of matrices R^{1k} are depended on t and can be calculated in symbolic mode [6]. But such algorithms are quite complex. In this paper a numerical implementaton of it is used. In this case matrices R^{1k} are evaluated in the specific time and presented as numerical matrices.

Symplectication

The relation (3) can be presented as map transformation

$$X = R \circ X_0. \qquad (4)$$

This map R is symplectic if

$$M^* J M = J, \forall X_0, \qquad (5)$$

where $M = \partial X/\partial X_0$ and M^* is the transponse of M, E is identity matrix,

$$J = \begin{pmatrix} 0 & E \\ -E & 0 \end{pmatrix}. \qquad (6)$$

Relation (5) in case of numerical matrices R^{1k} leads to a system of equations

$$a_0 + A_1 \mathbf{X_0}^{[1]} + \cdot + A_k \mathbf{X_0}^{[k]} = 0,$$

where A_i is a numerical vector. Note that this equation must be satisfied for any X_0. It means that the coefficients of each polynom are equal to zero and in this way appropriate corrections of the elements of the matrices R^{1k} can be found.

Map concatenation

Imaging we have two numerical serial maps that corresponds to the different systmes of ordinary differential equations

$$X_1 = \sum_{k=0}^{k_1} R_1^{1k}(t)X_0^{[k]},$$

$$X_2 = \sum_{k=0}^{k_2} R_2^{1k}(t)X_1^{[k]}.$$

Substituting X_1 to the equation for X_2 we obtain

$$X_2 = \sum_{k=0}^{k_1 \cdot k_2} \tilde{R}_2^{1k}(t)X_0^{[k]}.$$

As you can see the resulting map has order $k_1 \cdot k_2$. But we can use terms of order not higher than $max(k_1, k_2)$

SIMULATION OF ELECTROSTATIC STORAGE RING

Electrostatic storage ring consist of elements with different electric field distribution. In this research quadrupole lenses, cylindrical deflectors and drifts are used. The orbital motion and spin dynamics of the particle are described in [4]. Using these equations it is possible both serial tracking in each elements by step-by-step integration method and to build matrix form for each lattice element and concatenate it. In this research the 3 order of nonlinearity for resulting map is used. Moreover additionally correction of elements of matrices R for symplectic condition satisfying is completed. This symplectication procedure is performed once for map.

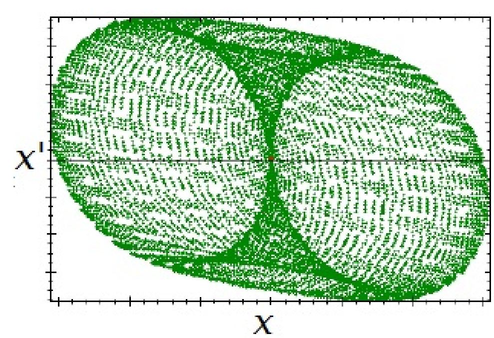

Figure 2: Step-by-step integration.

COMPARISON AND RESULTS

Comparing the results of calculations through single element good coincidence in computational model between matrix formalism approach and step-by-step integration was found out. However different approaches, methods of symplectication and so on introduces the calculation errors for the whole ring. In the article it proposed to use the comparison based on behavior of particles in predefined test cases.

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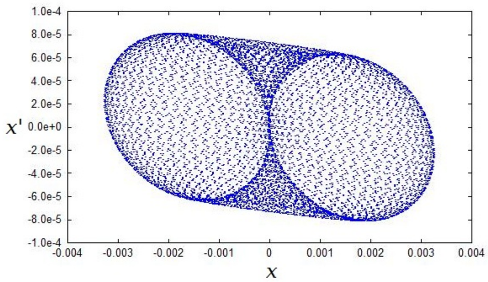

Figure 3: Matrix formalism

In Fig. 2 and 3 transverse plane of a particle (lattice with RF cavity) is presented. In these figures a particle motion with kinetic energy deviation in 310^{-4} and zero transverse displacement is shown. The similar correspondens in orbital motion of particles in longitudinal planes are also obtained.

For a numerical comparison spin coherence time (SCT) is used. SCT is the time of incogerent spin rotation on 2π rad, that is equal to the time during which the RMS spread of the spin orientation of all particles in the bunch reaches one radian.

Table 2: SCT, sec

Case	MF	Tracking	COSY Infinity
		RF = OFF	
$\Delta x = 3mm$, $\Delta k/k = 0$	1980	1418	3292
$\Delta x = 0mm$, $\Delta k/k = 10^{-4}$	0.301	0.243	323
		RF = ON	
$\Delta x = 0mm$, $\Delta k/k = 10^{-4}$	5813	5260	7316
$\Delta x = 0mm$, $\Delta k/k = 310^{-4}$	653	639	774

In Table 2 SCT in sec for different numerical approaches is shown. MF means mapping approach based on Matrix Formalism, tracking column corresponds to the step-by-step integration and COSY Infinity is a program for beam dynamics simulation based on map building by differential algebra concept. The results of simulation showed good agreement beetwen matrix formalism approach and step-by-step integration. SCT that was evaluated in COSY Infinity program differs from these results. It can be caused by different mathematical models, reference orbit designing and etc. Note, that for tracking approach and matrix formalism the same mathematical description of particle motion and spin dynamics was used.

CONCLUSION

The tracking approach is devoted to the high precesion step-by-step integration. On the other hand there are exist mapping algorithms for beam dynamic simulation. Such methods allows to build map corresponded to the dynamic system. Matrix formalism is a high performance approach for ordinary differential equations solving. Comparison of these two numerical methods shows good correspondes between them. So the matrix formalism can be succesfully used for long-term beam dynamics simulation.

We also plan to modify the given approaches for the direct calculation of the effect of EDM, fringe fields, etc., without significantly reducing of the calculation performance.

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