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IMPROVED TRACKING CODES : PRESENT AND FUTURE*

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1. SUMMARY AND INTRODUCTION

The paper identifies conditions which tracking codes should meet. The constraints come from mathematics, physics, computer environment and user requirements. There is no intention to do an exhaustive study of existing codes. Only single particle tracking codes are considered. When many particles are followed they have no interaction with each other. The paper ends with comments on present efforts to meet some of the conditions identified.

2. DEFINITION OF THE PROBLEM

The problem analyzed is the tracking of particles in beamlines and circular machines. The particles have a mass, a charge and are subjected to electromagnetic forces. Their motion is described with respect to a reference trajectory, within the scope of Hamiltonian Mechanics. The purpose of a tracking code is to produce numerical values for the coordinates of particles after they have been subjected repeatedly to the action of the electromagnetic elements which constitute the beam line. The errors affecting these numerical values should be small enough to draw meaningful conclusions. The speed of modern computers allows tracking through a great number of elements. The ease with which these computations are made tends to remove the user from the problem of computational error accumulation. These errors arise from simplifying assumptions made in the development of the mathematical model describing the physical situation, from the approximation with which solutions of the equations of the mathematical model are obtained, from the restricted number space on which the computers are operating. Sometimes the speed requirement entices the user to make assumptions or take shortcuts that lead to results which hide the true physical behavior.

3. THE MATHEMATICAL MODEL

Let us consider motion in three dimensional space and denote the coordinates by $q = (q_1, q_2, q_3)$. The motion of particles can be described by the hamiltonian equations

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \quad \dot{p}_i = -\frac{\partial H}{\partial q_i} \tag{1}$$

where p_i are the conjugate momenta of the variables q_i. H is the hamiltonian describing the system.

A point transformation $Q = Q(q,p,t)$ $P = P(q,p,t)$ is canonical when there exists a function K(Q,P,t) (new hamiltonian) such that the variables Q, P satisfy the equations:

$$\dot{Q}_i = \frac{\partial K}{\partial P_i} \quad \dot{P}_i = -\frac{\partial K}{\partial Q_i} \tag{2}$$

The functions Q and P satisfy the following conditions:

$$[Q_i, Q_j] = 0 \quad [P_i, P_j] = 0 \quad [Q_i, P_j] = \delta_{ij}$$

where $[a,b]$ is the Poisson bracket of a,b defined as :

$$[a,b] = \sum_j \left(\frac{\partial F}{\partial q_j}\frac{\partial G}{\partial p_j} - \frac{\partial F}{\partial p_j}\frac{\partial G}{\partial q_j} \right)$$

Given initial conditions for the variables q_i and the momenta p_i, a solution exists which can be written in the form :

$$q_i = q_i(q_{i0}, p_{i0}, t) \quad p_i = p_i(q_{i0}, p_{i0}, t) \tag{3}$$

The transformation, from the initial conditions to the values at time t, is a canonical transformation. Thus the functions q_i and p_i satisfy the following relations :

$$[q_i, q_j] = 0 \quad [p_i, p_j] = 0 \quad [q_i, p_j] = \delta_{ij}$$

or explicitly :

$$\begin{aligned} &\sum_{j0} \left(\frac{\partial q_i}{\partial q_{j0}}\frac{\partial q_k}{\partial p_{j0}} - \frac{\partial q_i}{\partial p_{j0}}\frac{\partial q_k}{\partial q_{j0}} \right) = 0 \\ &\sum_{j0} \left(\frac{\partial p_i}{\partial q_{j0}}\frac{\partial p_k}{\partial p_{j0}} - \frac{\partial p_i}{\partial p_{j0}}\frac{\partial p_k}{\partial q_{j0}} \right) = 0 \\ &\sum_{j0} \left(\frac{\partial q_i}{\partial q_{j0}}\frac{\partial p_k}{\partial p_{j0}} - \frac{\partial q_i}{\partial p_{j0}}\frac{\partial p_k}{\partial q_{j0}} \right) = \delta_{ik} \end{aligned} \tag{4}$$

Let us consider the six dimensional vector

$$v = (q_1, p_1, q_2, p_2, q_3, p_3)$$

and the Jacobian of the transformation (3):

$$M = \begin{pmatrix} \frac{\partial q_1}{\partial q_{10}} & \dots & \frac{\partial q_1}{\partial p_{30}} \\ \dots & \dots & \dots \\ \frac{\partial p_3}{\partial q_{10}} & \dots & \frac{\partial p_3}{\partial p_{30}} \end{pmatrix}$$

The conditions (4) can be expressed in terms of the matrix M as follows :

$$MJM^t = J \tag{5}$$

Where J is the matrix :

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \end{pmatrix}$$

and M^t is the transpose of M. The condition (5) is called the symplectic condition. All solutions to hamiltonian equations

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must satisfy this condition. Conversely if a transform (3) satisfies the conditions (5) then there exists locally a hamiltonian and a set of associated hamiltonian equations to which (3) is a solution.

Let us now give some examples to illustrate the importance of the previous conditions and how they are met in practice.

A. First Order Solution to the General Equations of Motion.

We adopt the definition of first order given in Ref. 1. With this definition the functions q_i and p_i are linear functions of the initial conditions. The transfer matrix M is constant. Thus if matrix M satisfies the symplectic condition it will be symplectic for all values of the input variables. Because of this property, the symplectic condition is always easy to satisfy in programs limited to first order.

B. The Impulse Approximation of Electromagnetic Elements.

When the transverse motion of a particle within an element is very small compared to the average transverse motion in a beamline, we may approximate the motion within that element and assume that the transverse coordinates of the particle remain unchanged. The Eqs. (3) become:

$$q_i = q_{i0} \qquad p_i = f_i(q_{j0}) + p_i \tag{6}$$

Contrary to a common belief, the Eqs. (6) do not generally satisfy the symplectic condition. The functions f_i must satisfy the following relations:

$$\frac{\partial f_i}{\partial q_{j0}} = \frac{\partial f_j}{\partial q_{i0}} \tag{7}$$

These conditions are obviously satisfied if each f_i is a function of the variable q_{i0} only.

The correct impulse approximation of the electromagnetic multipole kicks does satisfy the symplectic condition. Note that the variables q_i and p_i are canonical sets. A program whose transforms are symplectic may not represent hamiltonian motion if its variables are not canonical.

C. Higher Order Approximations.

Generally the solution (3) is a set of analytic functions which can be approximated by polynomials of degree n. The terms of the transfer matrix M are polynomials of degree $n-1$. The left hand side of the condition (5) is of degree $2n-2$; it will, usually, be satisfied only to degree $n-1$ because the terms of degree higher can only cancel with the corresponding terms of the matrix M and of the matrix M^t. Thus the truncated solution of degree n is symplectic only to degree n and generally is NOT symplectic to all orders.

H.Thiessen[2] observed that this departure from the symplectic condition could lead to numerical phenomena which do not represent any physical motion. Figure 1, extracted from,[3] shows such a case where Liouville theorem is clearly violated. It is the author's experience that, to second order, this has been observed only in lattices containing dipoles with strong quadrupole and sextupole components. The effect disappears when one extracts the quadrupole and sextupole components from the dipole magnets and replaces them by separate magnets.

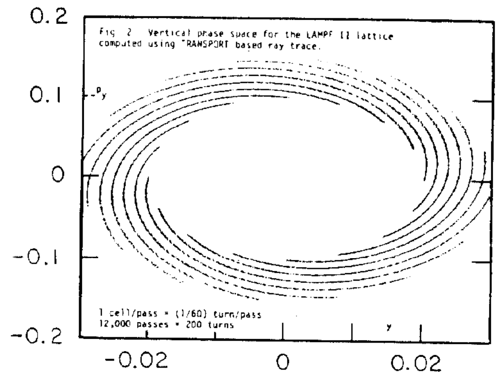

Figure 1: Transform symplectic to second order.

D. Symplectification.

Approximations are inevitable. Does there exist a procedure to create a transformation which is symplectic to all orders and whose truncation to order n coincides with the approximation defined in C.? Using the Lie Algebraic approachEtienne Forest[4] first developed a procedure which demonstrated that the symplectification of the transformation did cure the problem observed with standard tracking programs. This feature has been introduced in the program MARYLIE[5] and the program DIMAT.[6]

Figure 2 shows that after correction for symplecticity there is no indication of invariant violation.

A note of caution here is in order. There are simple, symplectic transformations which display chaotic behavior. Such behavior obviously cannot be removed by the symplectification process. Neatness of a phase plot is not a necessary condition for symplectic behavior. We shall come back to this point when talking about concatenation.

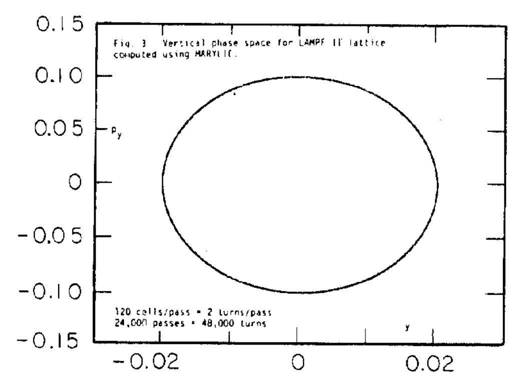

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Figure 2: Second order transform, symplectic to all order.

E. Subdivision of Elements.

The departure of any approximation from the exact solution of the equations of motion is an error of some order. The obvious simple way to reduce this error is to split the electromagnetic element in subelements and trace the particles successively through the subelements. This is like reducing the step size of a differential equation solver to increase accuracy. This method also cured the problem displayed in Fig. 1. In all cases, the removal of the problem occurs at the expense of computing time.

4. NUMERICAL SOLUTION

The equations of motion (1) can be solved by numerical procedures like the Runge-Kutta differential equation solvers. These procedures are affected by errors due to the order of the solver, to the choice of the step size and to the fact that the solution provided by the solver is usually not symplectic beyond the approximation error. Thus these numerical procedures can be affected with diseases similar to that of figure 1. Some solutions to this problem are:

a) Find new solvers that are symplectic to all orders.

b) Find solvers of greater order than the standard RK4-4 solver.

c) Reduce the stepsize sufficiently so that the errors lie in the range of the round off errors of the computer being used.

A. R. RUTH[7] introduced the first symplectic solvers directly based on the hamiltonian formalism.

B. When tracking particles in magnets one does not generally need to know the position of particles inside the magnet. There exists self starting Runge Kutta solvers that provide very accurate solutions to the equations of motion with large step sizes and with less function calls. They have been successfully used at the early stages of the design of the ring EROS. Some of these solvers can be found in Ref. 9.

Fast equation solvers based on perturbation theory of hamiltonian mechanics are being developped by Ruth and Warnock[8]

C. The third approach is similar in nature to the one presented in paragraph 3 E. Whatever the solver chosen (the second order transport matrix may be considered as a solver of the equations of motion) computational errors can always be decreased by reducing the stepsize of the computation, until the level of the roundoff errors is reached.

5. COMPUTER LIMITATIONS

As far as we are concerned the limitations due to the computer are of three types

a) The number system used by the compilers.

b) The memory space available under direct access.

c) The time to execute the tracking.

A. The final aim in particle tracking is the obtention of numerical values for the coordinates of the particles. The ultimate precision is bound by the number system used by the compiler, it characterizes the roundoff errors. At this level the solutions are no longer symplectic and if severe conditions are created and the particles are tracked through enough elements, non physical effects will be observed. The determination of the progression of roundoff errors is a complex problem. One way to put it in evidence is to switch to a higher precision structure in the computer hardware or software and observe the differences. Another way is to track the particles backwards through the elements (without doing an exact mathematical inversion). The observed differences are a measure of the roundoff errors. The above comments show that, no matter what, we are limited ultimately by the computer software structure and in the final analysis by the amount of time we are willing to spend on a given problem.

B. The memory requirement and the execution time are closely linked. Parallel processors are a great help in this respect. An imaginative effort is taking place at DESY.

With the intent to track many particles over a few hundred thousand turns around the machine HERA, Wrülich[10] has suggested to assemble a great number or microprocessors in parallel. Each microprocessor will track one particle. The data needed by the micros is processed by a mainframe unit.

C. To save time many users resort to concatenation. Concatenation is the grouping of many elements together and representing them by one transform of some order. For example in the second order matrix formalism a subsection of a lattice would be represented by a single matrix. In the Lie algebraic approach the subsection would be represented by a polynomial of some order. This procedure definitely improves the time performance but is not devoid of dangers.

Depending on the problem, concatenation will definitely hide some behavior and will alter details of chaotic motion. For the detailed analysis of the extraction process from the EROS pulse stretcher it was found that no concatenation was allowed.[11]

6. MAXWELL'S EQUATIONS REQUIREMENTS

The fields, through which the particles drift, satisfy Maxwell equations.As with the solution to the equations of motion (1), the solution to the Maxwell equations can be expressed as a polynomial expansion(see Ref.[12]). In the case of a static magnetic field with midplane symmetry defined by the gradient of the potential ϕ we obtain:

$$\begin{aligned}\nabla^2\phi = &\frac{1}{(1+hx)}\frac{\partial}{\partial x}\left((1+hx)\frac{\partial\phi}{\partial x}\right)\\ &+\frac{\partial^2\phi}{\partial y^2}+\frac{1}{(1+hx)}\frac{\partial}{\partial s}\left(\frac{1}{(1+hx)}\frac{\partial\phi}{\partial s}\right)=0\end{aligned} \tag{8}$$

$$\begin{aligned}\phi(x,y,s) =&(A_{10}+A_{11}x+A_{12}(x^2/2!)+A_{13}(x^3/3!)+\cdots)y\\ &+(A_{30}+A_{31}x+A_{32}(x^2/2!)+\cdots)y^3/3!+\cdots\\ =&\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}A_{2m+1,n}\frac{x^n}{n!}\frac{y^{2m+1}}{(2m+1)!}\end{aligned} \tag{9}$$

$$\begin{aligned}A_{30} =& -A''_{10}-A_{12}-hA_{11}\\ A_{31} =& -A''_{11}+2hA''_{10}+h'A'_{10}-A_{13}-hA_{12}+h^2A_{11}\\ A_{32} =& -A''_{12}+4hA''_{11}+2h'A'_{11}-6h^2A''_{10}-6hh'A'_{10}-A_{14}\\ &-hA_{13}+2h^2A_{12}-2h^3A_{11}\\ A_{33} =& -A''_{13}+6hA''_{12}+3h'A'_{12}-18h^2A''_{11}-18hh'A'_{11}\\ &+24h^3A''_{10}+36h^2h'A'_{10}-A_{15}-hA_{14}+3h^2A_{13}\\ &-6h^3A_{12}+6h^4A_{11}\end{aligned} \tag{10}$$

The above recursion relations show that when one truncates the polynomial expansion to some degree, then Maxwell equations are generally verified up to that order only (when the curvature is not zero or when the field vary along the longitudinal dimension). In conclusion the truncation of the field expansion creates a representation of the fields which do NOT satisfy Maxwell equations. In this case, however, there is no simple fix like we had for the symplectic condition.

The choice of a coordinate system,in which Maxwell equations variables separate, provides solutions in the form of a series expansion of eigenfunctions. An example of this approach is given in Ref. 9. We reproduce the expressions for the static magnetic field in a multipole element (not containing a dipole term).

$$\begin{aligned} B_x &= \sum r^{n-1}[-(b_n z + \beta_n)\cos(n-1)\phi \\ &\quad - (a_n z + \alpha_n)\sin(n-1)\phi] \\ B_y &= \sum r^{n-1}[(b_n z + \beta_n)\sin(n-1)\phi \\ &\quad - (a_n z + \alpha_n)\cos(n-1)\phi] \\ B_z &= \sum \frac{r^n}{n}(-b_n \cos n\phi - a_n \sin n\phi) \end{aligned} \tag{11}$$

Equations (11) are expressions for constant or linearly varying fields along the longitudinal axis z. A similar set of equations is obtained for fields with a general longitudinal variation (see details in Ref. 9). The powers of r are replaced by Bessel functions and the linear dependence in z by a sum of cosine and sine terms.

In both cases Maxwell equations are satisfied to all orders, whatever the truncation point. To economize computer time, a multipole can be divided in three parts: a central constant field part surrounded by fringing field zones. But,in this process, one always creates some discontinuity in the value of the fields or of some derivative at the joining surface between the zones. One can represent adequately the multipole as one unit but at the expense of computing time. The author does not know of a similar representation for the fields of a dipole magnet with respect to the reference trajectory.

Another method of representing the fields is with the help of a field map. Field values are obtained by interpolation.They must be accurate enough so that Maxwell equations are satisfied to the roundoff precision of the machine.

7. USER REQUIREMENTS

The user needs more than one program because of the complexity of the problems at hand. Also the research field is in permanent evolution and new ideas need be tested and applied. This demands that tracking and design programs have user friendly input facilities and be compatible with each other.Last year under the inspiration and direction of Carey and Iselin[13] a standard input format was introduced and hopefully it will be adopted internationally. But that is not enough. All programs should not have to go through repeated fitting procedures of a preliminary design. A standard data base must be defined which existing or future programs can access to perform studies of already designed lattices.J. Niederer and F. C. Iselin[14] are directing efforts in this area.

8. CONCLUSIONS

It is the author's opinion that all tracking and design codes meet the following requirements:

1. Use of standard input format.
2. Use of canonical variables only and as defined in the standard input format.
3. The symplectic condition to the order of the program is satisfied.
4. Option to guarantee symplecticity to all orders.
5. Correct definition of the electromagnetic fields up to the order of the solution of the equations of motion, including the fringe fields with their longitudinal components.
6. Concatenation is available with a warning of caution.
7. Possibility to create or use the standard data base.

There is not a single tracking code that satisfies all these requirements. Within the framework of the design efforts for LEP,HERA,SLC,SSC (to name but a few projects) a number of researchers are attempting to meet some of these requirements. The initial impetus stems from the work of Iselin[16] at CERN. Other programs that follow or will follow the trend set in MAD[16] are: COMFORT,[15] MARYLIE,[5] PATRICIA,[17] SYNCH,[18] DIMAT (in its version DIMAD),[22] HARMON,[19] TRANSPORT[20] and TURTLE.[21]

The previous list does not pretend to be exhaustive.

To conclude, the spectre of the need to satisfy the symplectic condition was a non-issue. There are many, equally valid, simple solutions to the problem. Most programs are meeting this condition or will do so in the near future.

Efforts should be concentrated on adequate and practical definition of the fringing fields. When all factors of time,space and accuracy are considered, the best approach will probably be the direct solution of the differential equations of motion with new fast solvers. The most difficult problem at present, is the simple and practical definition and representation of fringing fields in dipole magnets.

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