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ROUNDING ERRORS IN BEAM-TRACKING CALCULATIONS

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The computer simulation of particle dynamics in accelerators and storage rings has become an important tool in accelerator physics. In one method particles are tracked by explicitly computing their motion through the magnets and the drift spaces of the machine ("kick codes"). The purpose of our work is to investigate how the results are affected by the finite numerical accuracy of the computation. Our study reveals a strong influence of rounding errors on the results of tracking calculations. They grow much more rapidly with the number of turns than naively expected. Therefore they give a limit of meaningful calculations. In our example, this limit is reached for a few 10^6 turns around the storage ring, corresponding to some 10 seconds' real-storage time.

I. INTRODUCTION

At DESY an electron-proton collider HERA (hadron-electron ring accelerator) will be built. It will consist of two separate storage rings for the electrons and protons. The proton ring will have superconducting magnets. The proton storage ring was used as an example in the present investigation. Particles were tracked by explicitly computing their motion through the magnets and drift spaces of the machine. The motion of a particle in the magnetic field of a storage ring is described by the following differential equations:

$$\begin{aligned} \frac{d^2x}{ds^2} + K_x(s) \cdot x &= \frac{e}{p_0} \cdot B_z(z, x, s), \\ \frac{d^2z}{ds^2} + K_z(s) \cdot z &= -\frac{e}{p_0} \cdot B_x(z, x, s), \end{aligned} \tag{1}$$

where

x, z = horizontal and vertical displacement of the particle from the ideal orbit,
s = longitudinal coordinate,
K_x, K_z = focusing strengths (including weak and edge focusing),
B_x, B_z = transverse components of the additional magnetic field ($B_s = 0$),
p_0 = design momentum of the particle.

The actual computation was done using the program RACETRACK[1]. We investigated the role of rounding errors using this program as applied to one version of the HERA proton storage ring. In the RACETRACK code linear magnetic elements (drift spaces, dipoles, quadrupoles) are represented by their transformation matrices. These elements are combined into blocks as far as possible. Each block is represented by one matrix only. The coordinates after the kth block are calculated by the usual matrix formalism for linear optics. Nonlinear elements are treated in the thin-magnet approximation. This means that only the direction of the particle (x', z') is changed at one point in the middle of the magnet ("kick code"):

$$x'_{k+1} = x'_k + \Delta x',$$
$$\Delta x' = \frac{l}{\rho} \cdot \sum_{n=1}^{9} (b_n + ia_n)(x + iz)^{n-1}. \tag{2}$$

In the HERA structure, which we have used for our investigations,[2] we had 836 linear blocks, 208 pure sextupoles, and 600 elements with multipoles up to and including $n = 9$.

The polynomials in Eq. (2) were developed by hand and explicitly written down as "Horner Schema" in the computer code. To calculate one turn around the storage ring, we had to carry out 250 000 floating-point operations. Normally the calculations are carried out in double precision on an IBM 3081 computer. In this case, one revolution, which corresponds to 20 μs storage time, takes 80 ms of CPU time. Much of this work was also done on a 370 E (emulator), developed by H. Brahman *et al.* (Weizmann Institute) and operated at DESY by D. Notz. Its speed is about 1/5 of an IBM 3081D for our codes.

On an IBM computer, single-precision numbers are represented with 24-bit mantissa, double precision with 56, and fourfold precision with 120-bit mantissa. The error in the representation of a single number, the single roundoff error, is of the order of 2^{-t} for a t-bit mantissa; for IBM computers it may be up to a factor of 8 larger because of their hexadecimal normalization.

So, single rounding errors are very small, but they propagate and accumulate and therefore become non-negligible after some time.

II. METHODS

We have used three different methods to determine the size of rounding errors.

The first method can only be applied for the special case of linear optics without skew quadrupoles. Here the horizontal coordinates x, x' and the vertical coordinates z, z' are independent of each other. The emittance

$$\varepsilon_x = \frac{1}{\beta(s)} \cdot \left\{x^2(s) + \beta^2(s) \cdot \left[x'(s) + \frac{\alpha(s)}{\beta(s)} \cdot x(s)\right]^2\right\} \tag{3}$$

(and ε_z analogous) is a constant of motion. β is the β-function and $\alpha = -\frac{1}{2}\frac{d\beta}{ds}$. The emittance can be calculated from the starting coordinates and must remain constant as the particle is traced through the lattice. Deviations must be due to rounding errors.

In a second general method the rounding error can be determined by comparing the tracking results with those of a much more accurate reference calculation. Comparison of single precision with a double-precision reference does not work, because single precision is much too inaccurate to be of any practical value. So we emulated a 40-bit mantissa (by masking the last 16 bits of double precision with zeros after each floating-point operation). The results of this calculation were compared to a double-precision reference. We have checked by a calculation with fourfold precision that this reference is good enough for our purpose.

As a third method we used backtracking. The particle is first tracked for a number of turns N around the ring. Then its direction is reversed, and it is traced back through the same magnet structure. It should then go exactly the same way back and finally after N turns of backtracking be at the starting point again. Failure to do so must be due to the influence of rounding errors during the calculation of a total of $2N$ revolutions. We determined the rounding error for smaller numbers of revolutions by looking at corresponding points along the path of the particle: on its way back, the particle should go through the same points it went through forward. The distance of these corresponding points is due to rounding errors.

For the backtracking, the matrices of the linear optics are inverted:

$$\mathbf{M}=\begin{pmatrix} a & b \\ c & d \end{pmatrix}, \qquad \mathbf{M}^{-1}=\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}, \tag{4}$$

because $\det \mathbf{M}=1$. The kick $\Delta x'$ is calculated in the same way as for the tracking, but it is subtracted, not added.

As a check, we compared the results of the three methods for a linear machine (the HERA proton ring without sextupoles and higher-order multipoles).

We have chosen 10 particle trajectories with starting coordinates lying on a phase-space ellipse with a betatron amplitude of 12 mm at the starting point.

After averaging over the 10 particles, we found the following results: as expected, the errors for 40-bit accuracy are larger by a factor of 2^{16} than the errors for 56-bit accuracy.

The relative errors of z and z' are roughly equal; therefore for 40-bit accuracy we calculated a common mean value. The relative error of the emittance is about a factor of two greater than the one of the coordinates. This fact is roughly expected from Eq. (3). These results are shown in Fig. 1.

In summary, the three different methods give a consistent picture for the linear machine. In the same sense, we compared in spot checks the two applicable methods for the nonlinear machine and got consistent results.

III. RESULTS

We used the program RACETRACK as described to test the effect of rounding errors on the result of tracking calculations. We used the method of backtracking and double precision (real $*$ 8, 56-bit mantissa).

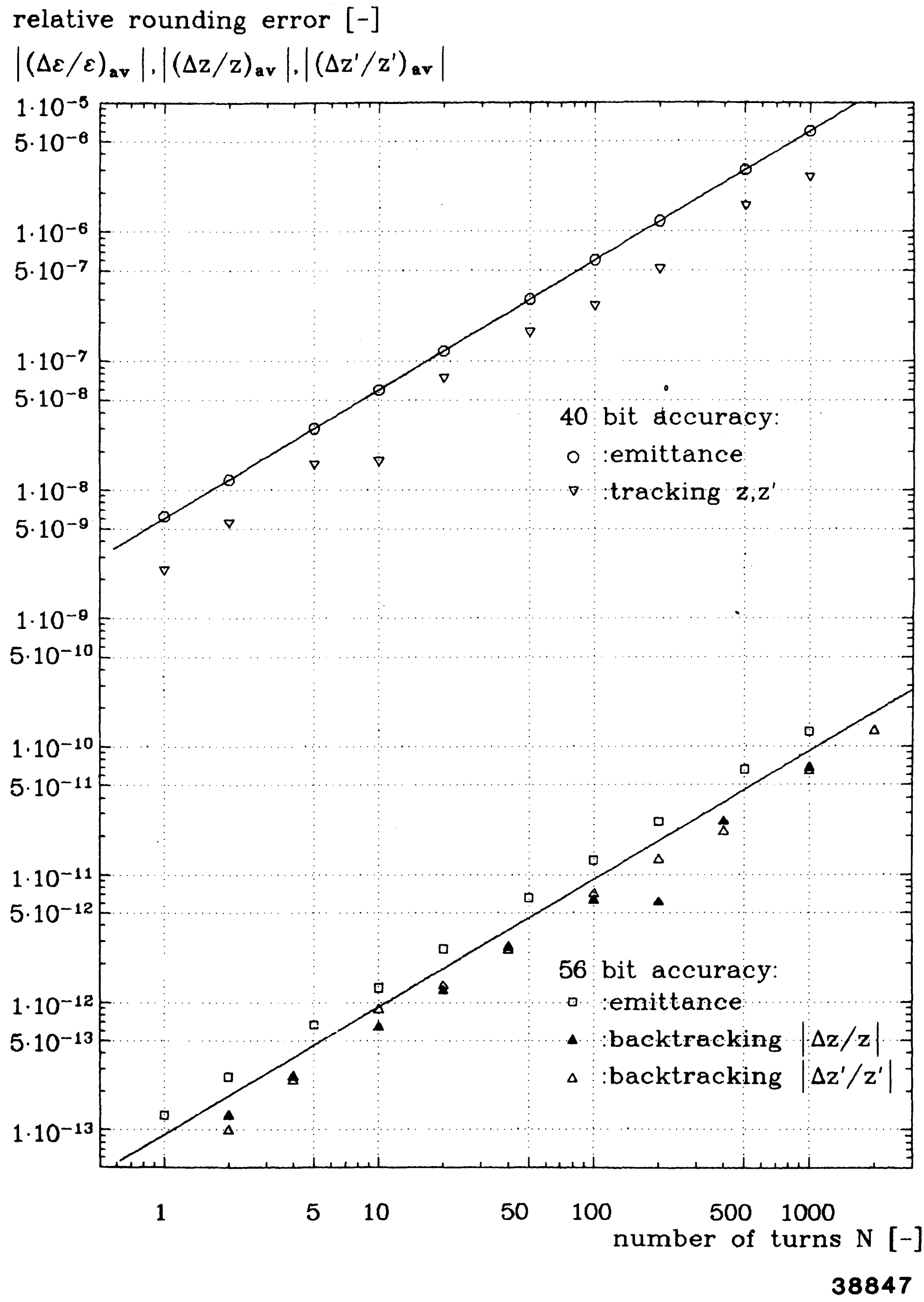

FIGURE 1 Relative rounding errors for tracking as functions of the number of turns (for 40-bit and 56-bit accuracy).

We first studied the linear machine (only dipoles, quadrupoles, and drift spaces). We find that the relative error increases roughly proportional to the number of revolutions N, see Fig. 1. We plotted the distribution of the relative rounding errors in Fig. 2.

There are two groups of entries: the errors in the horizontal (x, x') and vertical (z, z') coordinates, respectively. The average error in each group grows approximately linear with N. This behavior can be understood from the nature of the linear approximations.

Consider the transfer matrix $\mathbf{M}$ for one complete revolution around the ring, obtained by multiplying all individual transfer matrices together. We should have $\det \mathbf{M} = 1$, and this guarantees that the emittance ε is a constant of motion. Due to rounding errors, the matrix $\mathbf{M}'$ actually used in the calculations does generally not have $\det \mathbf{M}' = 1$. Depending on whether $\det \mathbf{M}' \gtrless 1$, the emittance will increase/decrease with each turn, leading in the average to a positive/negative value of the error. Since the same (wrong) matrix is used for each turn, this effect accumulates with the same sign for each turn, and the error increases linearly with N. It therefore prevails over the effect of random rounding errors, which should grow like $N^{1/2}$.

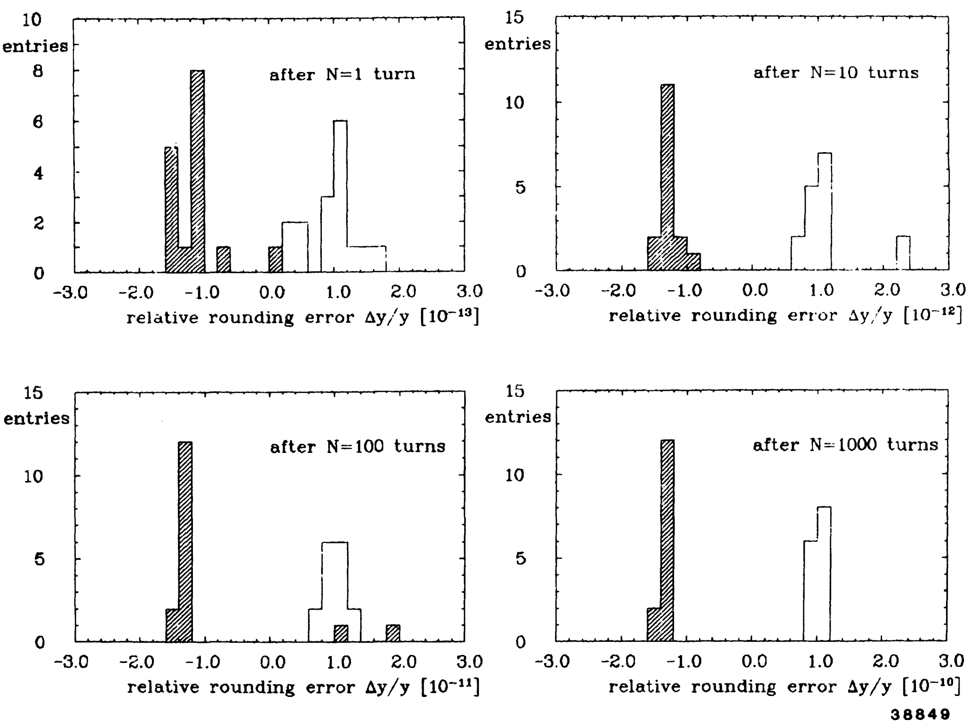

FIGURE 2 Evaluation of relative rounding error for particles with $x_{\max} = 1.2\,\mathrm{cm}$ in the linear machine. Note change of scale.

unshaded: $y = x, x'$; $\det \mathbf{M}' - 1 = 1.2 \cdot 10^{-13}$

shaded: $y = z, z'$; $\det \mathbf{M}' - 1 = -0.8 \cdot 10^{-13}$

This behavior is borne out in Fig. 2. As a matter of fact, the two coordinate groups x, x' and z, z', which are calculated independently of each other, differ in the sign of $(\det \mathbf{M} - 1)$. It should be noted here that the determination of the sign of $(\det \mathbf{M} - 1)$ requires a calculation with fourfold precision (real*16).

For the nonlinear machine we investigated the absolute errors of the amplitudes and directions, normalized to their maximum value, determined in the linear machine.

We looked at the distributions of the normalized errors for samples of particle trajectories; they were chosen with the starting coordinates lying on phase-space ellipses with different betatron amplitudes.

The distributions are centered around zero and symmetric. The rms values $\left\langle \left(\frac{\Delta y}{y_{\max}} \right)^2 \right\rangle^{1/2}$ are plotted vs. the number N in Fig. 3. For large values of N the rms errors grow like N^2.

There is a strong dependence on the betatron amplitude. This behavior can be understood from the physics of a nonlinear storage ring, which determines the error propagation.

The betatron phase of a particle trajectory grows by $2\pi \cdot Q$ every turn, with Q = betatron tune. In the nonlinear machine, the tune Q depends on the betatron amplitude $x_{\max}$ according to

$$Q = Q_{\text{lin}}(1 + qx_{\max}^2)$$

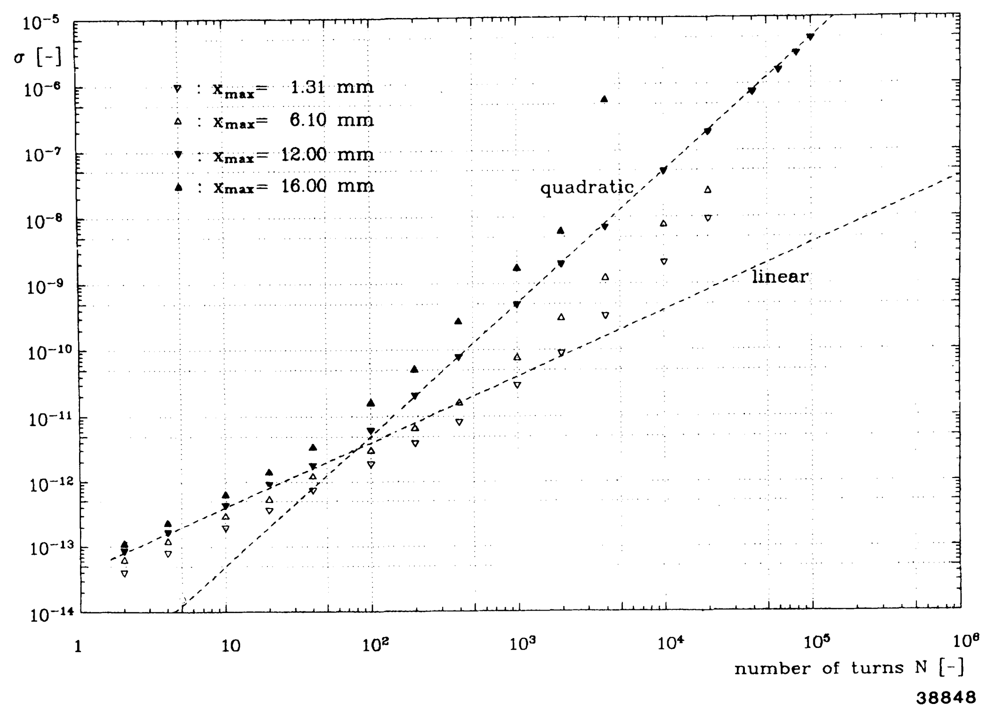

FIGURE 3 σ of normalized rounding error $\Delta y/y_{\max}$ for the nonlinear machine.

in first approximation. ($Q_{\text{lin}} = Q$-value of the linear machine, $q = \text{constant}$). Because of the determinant error, the amplitude changes systematically by $a \cdot x_{\text{max}}$, $a \simeq 10^{-13}$ every turn, so the computed value of x_{max} is

$$x_{\text{max}}^{\text{calc}} = x_{\text{max}}(1 + aN).$$

Therefore Q changes systematically every turn, and the error in tune will be

$$Q_{\text{calc}} - Q = Q_{\text{lin}} \cdot q \cdot x_{\text{max}}^2(2aN + a^2N^2).$$

For $aN \ll 1$ we can integrate this equation to get the error in betatron phase:

$$\begin{aligned}\phi^{\text{calc}} - \phi &\simeq \int_0^N 2\pi Q_{\text{lin}} q x_{\text{max}}^2 \cdot 2aN\,dN \\ &\simeq 2\pi Q_{\text{lin}} \cdot q \cdot x_{\text{max}}^2 \cdot a \cdot N^2,\end{aligned}$$

which shows indeed the N^2 dependence and the strong dependence on x_{max}. Our data reveal in fact that the error in phase is systematic in nature: error distributions in ϕ are again not centred around zero, but the sign of the error corresponds to the sign of the determinant error, indicating that the present interpretation is basically correct.

The significance of these observations is the following: Even though the magnitude of a single rounding error is very small, their accumulated effect grows with N^2 and will eventually overtake other effects which grow more slowly with N. For our problem rounding errors limit the possibility of meaningful tracking to a few million revolutions. However, the systematics explained above open the possbility to heuristically correct for those effects.[3]

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