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ON COORDINATE SYSTEMS IN BEAM DYNAMICS

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Abstract

Any description of the beam dynamics calculation and simulation relies on the proper choice of a coordinate system in order to minimize the computational complexity and to apply different level of approximations in the calculations. This need generates a large number of reference systems, especially to describe the longitudinal dynamics of a particle beam like (z, z'), $(t, \frac{\Delta P}{P})$, (z, ϕ), etc. In this paper we summarize the rules to change coordinate systems, which system is canonical and how the Hamiltonian of the beam transforms according to the chosen coordinate system.

INTRODUCTION

The literature of accelerator physics simulation codes is rich of different algorithms used to track charged particles in different kind of reference frames. Just to give some examples, we will describe here few common simulators.

MAD-X [1] uses $x, \frac{p_x}{p_0}, y, \frac{p_y}{p_0}, -c\Delta t, \frac{\Delta E}{cp_0(1+\frac{\Delta p}{p_0})}, s$, with x, y, p_x, p_y canonical coordinates and momenta, p_0 reference momentum, Δt time difference of the particle with respect to the reference particle, Δp momentum difference of the particle with respect to the reference particle and s, as independent variable, as arc length along the reference orbit.

TraceWin [2] uses $x, \frac{dx}{ds}, y, \frac{dy}{ds}, z, \frac{\Delta p}{p_s}, s$ with p_s the momentum in the direction tangent to the trajectory of the reference particle s.

IMPACT exists in two versions, depending on the coordinate systems, IMPACT-Z [3] uses $x, p_x, y, p_y, t, p_t, z$ where t is the time, and $p_t = -E$ the negative energy. z is the longitudinal coordinate. IMPACT-T [4] uses $\frac{x}{dz}, \frac{p_x}{mc}, \frac{y}{dz}, \frac{p_y}{mc}, \frac{z}{dz}, \frac{p_z}{mc}, t$ where $dz = cdt$ and $p_i = \gamma\beta_i$ with $i = x, y, z$.

PyORBIT [5] is agnostic about the coordinate system (can work in different ways if specified) but the default is the same coordinate system as TEAPOT [6] simulator, that uses the coordinate system of the old version of MAD [7] that is $x, \frac{p_x}{p_0}, y, \frac{p_y}{p_0}, -c\Delta t, \frac{\Delta E}{cp_0}, s$.

OpenXAL [8] uses $x, \frac{dx}{ds}, y, \frac{dy}{ds}, z, \frac{1}{\gamma^2}\frac{\Delta p}{p}, s$, like TraceWin but scaled with a γ^2 Lorentz factor in the longitudinal momentum.

From this list it seems that the choice of coordinate system is arbitrary and there is a large freedom to select the frame for simulation but what are the base criteria to chose one? In the following sections we will try to give a general guideline in the properties that a reference system has to fulfill, in order to be suitable for a simulator in accelerator physics.

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CANONICAL TRANSFORMATIONS

Regardless of the particle accelerator that we want to simulate, we can start from an assumption that is always valid: the physics of our simulator will be derived from the Hamiltonian

$$H = c\sqrt{\left(\vec{p} - e\vec{A}\right)^2 + m^2c^2} + e\phi \tag{1}$$

where the potentials $\vec{A}$ and ϕ are such that the corresponding fields are

$$\vec{E} = -\vec{\nabla}\phi; \quad \vec{B} = \vec{\nabla} \times \vec{A} \tag{2}$$

plus the usual gauge freedom; e is the electric charge; m is the mass of the particle; c is the speed of light. Such Hamiltonian is valid because it produces the Lorentz force[1] that was extensively verified experimentally.

The equations of motion generated by the Eq. (1) are generally difficult to solve and a common trick is to consider the Taylor expansion of the Eq. (1) (the so-called paraxial approximation). In order to be able to expand around zero, the coordinates and momenta involved in the Hamiltonian have to be small, this is the reason why every particle accelerator code express the dynamics with respect to a "reference particle" that corresponds most of the time with the centroid of the bunch.

The Hamiltonian is a function of coordinates q_i and momenta p_i such that when evaluated on a particular time trajectory, it satisfies the differential equations

$$\dot{q}_i = \frac{\partial H}{\partial p_i}; \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}. \tag{3}$$

We expect that when we transform the q_i or the p_i we will obtain a new Hamiltonian that will satisfy a new set of Eqs. (3). This is assured by the canonical transformations, and for a full discussion the best reference is [10]. Here we will just explain the fundamentals.

Let us assume that a particle has coordinates q and momenta p, and that the motion during a certain time t satisfies the equations of Hamilton (3) of a certain Hamiltonian $H = H(q, p, t)$. Now we want to find the new Hamiltonian $K = K(\tilde{q}, \tilde{p}, \tilde{t})$ that satisfies the same set of equations in the new coordinate system $\tilde{q} = \tilde{q}(q, p, t), \tilde{p} = \tilde{p}(q, p, t), \tilde{t} = \tilde{t}(q, p, t)$.

$$\begin{tikzcd} t\,\mathbb{R} \arrow[r, "{(q,p,t)}"] & \mathbb{R}^{2n+1} \arrow[r, "H"] \arrow[d] & \mathbb{R} \arrow[d, equal, "id"] \\ \tilde{t}\,\mathbb{R} \arrow[u, "\phi"] \arrow[r, "{(\tilde{q},\tilde{p},\tilde{t})}"] & \mathbb{R}^{2n+1} \arrow[r, "K"] & \mathbb{R} \end{tikzcd} \tag{4}$$

[1] a proof that the classical version of this Hamiltonian generates the Lorentz force is available in [9]. For the relativistic Hamiltonian the calculation is the same but a bit longer.

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We evaluate $\frac{d\tilde{q}}{d\tilde{t}}$ as

$$\frac{d\tilde{q}}{d\tilde{t}} = \frac{\partial\tilde{q}}{\partial q}\frac{dq}{dt}\frac{dt}{d\tilde{t}} + \frac{\partial\tilde{q}}{\partial p}\frac{dp}{dt}\frac{dt}{d\tilde{t}} + \frac{\partial\tilde{q}}{dt}\frac{dt}{d\tilde{t}} \tag{5}$$

and the calculation is similar for $\frac{d\tilde{p}}{d\tilde{t}}$ and $\frac{d\tilde{t}}{d\tilde{t}}$, so we have

$$\begin{bmatrix} \frac{d\tilde{q}}{d\tilde{t}} \\ \frac{d\tilde{p}}{d\tilde{t}} \\ \frac{d\tilde{t}}{d\tilde{t}} \end{bmatrix} = \frac{dt}{d\tilde{t}} \begin{bmatrix} \frac{\partial\tilde{q}}{\partial q} & \frac{\partial\tilde{q}}{\partial p} & \frac{\partial\tilde{q}}{\partial t} \\ \frac{\partial\tilde{p}}{\partial q} & \frac{\partial\tilde{p}}{\partial p} & \frac{\partial\tilde{p}}{\partial t} \\ \frac{\partial\tilde{t}}{\partial q} & \frac{\partial\tilde{t}}{\partial p} & \frac{\partial\tilde{t}}{\partial t} \end{bmatrix} \begin{bmatrix} \frac{dq}{dt} \\ \frac{dp}{dt} \\ 1 \end{bmatrix}. \tag{6}$$

We also notice, from the diagram 4 that $H(q,p,t) = K(\tilde{q}(q,p,t),\tilde{p}(q,p,t),\tilde{t}(q,p,t))$ so we have

$$\begin{bmatrix} \frac{\partial H}{\partial q} \\ \frac{\partial H}{\partial p} \\ 1 \end{bmatrix} = \begin{bmatrix} \frac{\partial\tilde{q}}{\partial q} & \frac{\partial\tilde{p}}{\partial q} & \frac{\partial\tilde{t}}{\partial q} \\ \frac{\partial\tilde{q}}{\partial p} & \frac{\partial\tilde{p}}{\partial p} & \frac{\partial\tilde{t}}{\partial p} \\ \frac{\partial\tilde{q}}{\partial t} & \frac{\partial\tilde{p}}{\partial t} & \frac{\partial\tilde{t}}{\partial t} \end{bmatrix} \begin{bmatrix} \frac{\partial K}{\partial\tilde{q}} \\ \frac{\partial K}{\partial\tilde{p}} \\ \frac{\partial K}{\partial\tilde{t}} \end{bmatrix}. \tag{7}$$

The matrix in the Eq. (7) is the transposal of the matrix in the Eq. (6). If we call such a matrix J (as the Jacobian of the coordinate transformation) and we call S the matrix of the Hamilton equations extended with the additional row and column corresponding to the independent variable

$$\begin{bmatrix} \frac{dq}{dt} \\ \frac{dp}{dt} \\ 1 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial q} \\ \frac{\partial H}{\partial p} \\ 1 \end{bmatrix} = S \begin{bmatrix} \frac{\partial H}{\partial q} \\ \frac{\partial H}{\partial p} \\ 1 \end{bmatrix} \tag{8}$$

we finally have the condition that has to satisfy the transformation

$$\begin{bmatrix} \frac{d\tilde{q}}{d\tilde{t}} \\ \frac{d\tilde{p}}{d\tilde{t}} \\ 1 \end{bmatrix} = \frac{dt}{d\tilde{t}} JSJ^T \begin{bmatrix} \frac{\partial K}{\partial\tilde{q}} \\ \frac{\partial K}{\partial\tilde{p}} \\ 1 \end{bmatrix} = S \begin{bmatrix} \frac{\partial K}{\partial\tilde{q}} \\ \frac{\partial K}{\partial\tilde{p}} \\ 1 \end{bmatrix} \tag{9}$$

where the last equality is due to the new equations of Hamilton in the new coordinate system. This condition is a generalization of the usual symplectic condition for the case when the time is also transformed. It is easy to see that if $\tilde{t} = t$ the condition is exactly the symplectic.

The correct way to change the coordinates and preserve all the properties of the initial Hamiltonian (that should be the Eq. (1) because it generates the Lorentz force) is to apply a change of coordinates between the old and the new, such that the Jacobian of the transformation follows the rule of the Eq. (9). We will see in the next section that a large family of coordinate changes do not follow this rule.

INDEPENDENT VARIABLE TRANSFORMATIONS

One of the most used coordinate change in particle accelerators swaps the time with position. The assumption is that the particle beam moves mainly in the longitudinal direction, so the position and time are related with a transformation like

$$z = z_0 + \beta ct. \tag{10}$$

It is easy to prove that it does not exist any suitable change of coordinates that satisfies the Eq. (10) and the Eq. (9), so the Eq. (10) is not a canonical transformation. Then we should wonder if this transformation works and why. In order to apply the proper change of coordinates between position and time we have to go back to the action defined as [11]

$$A = \int_{t_1}^{t_2} L(q,\dot{q},t)dt \tag{11}$$

where $\dot{q} = \frac{dq}{dt}$ and L is the Lagrangian, the function of coordinates, velocities and time that maintains minimum (or maximum) the action A along the trajectory between t_1 and t_2.

The Hamiltonian is the Legendre transform of the Lagrangian defined as

$$p(q,\dot{q},t) = \frac{\partial L}{\partial\dot{q}} \tag{12}$$

$$H = \dot{q}p - L \tag{13}$$

where p is the conjugate momentum. Substituting this definition in the action we have

$$A = \int_{t_1}^{t_2} \left(\frac{dq}{dt}p - H\right) dt. \tag{14}$$

At this stage, it is possible to replace the time with the position applying the Eq. (10) with $z = q$ having

$$A = \int_{q_1}^{q_2} (\beta cp - H)\frac{dt}{dq}dq = \int_{q_1}^{q_2} \left(-H\frac{dt}{dq} + p\right) dq \tag{15}$$

where it was used the fact that $\frac{dt}{dq} = \frac{1}{\beta c}$.

The Eq. (15) says that we can treat our problem with a new set of assumptions and obtain the same action A. The assumptions are

$$\tilde{t} = q \tag{16}$$

$$\tilde{q} = t \tag{17}$$

$$\tilde{p} = -H \tag{18}$$

$$\tilde{H} = -p \tag{19}$$

with the new equations of Hamilton expressed in the new variables.

It is important to remark here that the swap of time with position produces a new Hamiltonian ($-p$) and this is the reason why it is not a canonical transformation. When a simulator applies a transformation that is not canonical, it is no longer using the Hamiltonian (1). This means that the new Hamiltonian should be verified experimentally because it may no longer produces the Lorentz force.

In the practical case of a time to position transformation operated through a constant factor (as it is βc in our example), we know from the measurements that everything works correctly but this is limited to the βc constant. In reality, we know that β can change in direction and value, especially when the particles are accelerated. Many simulators consider the acceleration in small steps or with the Transit Time

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Factor approximation (for the cavities) using the longitudinal position, as it is exactly like time. This approach tends to accumulate errors due to fact that the Eq. (15) is no longer simple for a β that changes in time, and the approximation of little steps could not work.

The most accurate way to simulate the dynamics of an accelerating particles is to maintain the Hamiltonian in the time domain not substituting time with space.

LONGITUDINAL VARIABLES

With the information about canonical transformation and change of variables in the action, we are ready to analyze the coordinate systems used in the particle dynamics codes.

The only code that uses a canonical transformation of the Eq. (1) is IMPACT-T because it uses time as independent variable. Such a simulator will then respect the Lorentz force even in the case of changes in the reference velocity (β_0).

The other analyzed codes use the position s, as independent variable, so they are applying the transformation (15), plus a canonical transformation of the new Hamiltonian to set a theoretical particle (the reference particle), as the center of coordinates and momenta. The longitudinal component of the generating function of type 2 used to do such a transformation is [11]

$$F_2 = \left(\frac{s_0}{\beta_0} - ct\right)\left(\frac{1}{\beta_0} + \tilde{p}\right). \tag{20}$$

The new conjugated variables for the longitudinal position and momentum are [11]

$$-c\Delta t; \quad \frac{\Delta E}{\beta_0 E_0} \tag{21}$$

with the zero index used for the reference particle. These conjugated variables can be transformed considering the relationship that exists between reference energy and reference momentum $E_0 = c\frac{p_0}{\beta_0}$

$$-c\Delta t; \quad \frac{\Delta E}{cp_0} \tag{22}$$

that is the coordinate system used by the default of PyORBIT, TEAPOT and the old version of MAD.

IMPACT-Z uses the same system but it sets to the unit the reference energy and velocity. This can be done safely because the action stays minimum even if the Lagrangian is scaled by a constant factor, but every time there is a change in the reference particle, this has to be included in a new scaling factor in the model.

The code that uses $\frac{\Delta p}{p}$ as longitudinal momentum are applying a different canonical transformation with the generating function

$$F_2 = (s_0 - \beta ct)\frac{(\tilde{p}+1)}{\beta}. \tag{23}$$

The conjugated variables for this transformation are

$$-\Delta z; \quad \frac{\Delta p}{p_0} \tag{24}$$

where $-\Delta z$ is commonly called z as in TraceWin. OpenXAL uses the same convention but it scales with a factor γ^2. This factor makes the longitudinal momentum equal to z' that is the angle of the tangential longitudinal vector with respect to the reference trajectory. This choice can simplify the calculations but at the price of evaluating all the equations from the forces and not from the Hamilton equations.

The last reference system that was not mentioned yet is the one of MAD-X that is similar to the one of TEAPOT but with an additional $\left(1 + \frac{\Delta p}{p_0}\right)$ at the denominator. This is due to a second order correction of the momentum expanded around the curvilinear reference trajectory as described in [12]. This coordinate system is non-canonical and requires a treatment evaluating the equations of motion from the forces.

CONCLUSIONS

We reviewed what is a general approach to canonical transformations and how to transform the Hamiltonian with a new coordinate system preserving the action. Then, we analyzed the longitudinal reference systems of the most common tracking code used in particle accelerators, evaluating which transformation was adopted and when this is canonical.

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