MOMENT METHODS FOR SIMULATION AND DESIGN*

Walter P. Lysenko
Los Alamos National Laboratory, Los Alamos, NM 87545

ABSTRACT

It is often advantageous to describe a particle beam by the moments of its phase-space distribution. This paper relates original work by Sacherer to presently-used linear design codes like TRACE3D and to some recent results.

INTRODUCTION

Beam behavior is often better described by the evolution of the phase-space distribution rather than by the single-particle motion. Consider a periodic beamline. It transports a matched beam with no change in the distribution. But the usual (single-particle) transfer maps contain a large number of entries (aberration coefficients) related to the complicated motion of the individual particles that obscure the simple nature of the evolution of the matched distribution. One way to describe a beam in terms of the phase-space distribution is by moments of this distribution. Such a description has two important features. First, the moments are closely related to observables such as beam positions (first moments) and sizes (second moments). Second, the moment approach is useful in simulations because only a small number of moments is required to describe a beam accurately to high order, a feature especially important in 3-D situations.

In 1971, Sacherer[1] presented his results based on the second-order moment equations, extending previous work on envelope equations by Kapchinsky and Vladimirsky[2]. Linear design codes like TRACE3D[3] make use of these results. Later, Paul Channell[4] proposed using the moment equations to higher order as the basis of a simulation code. Such a code was developed at Los Alamos[5]. Recent work on the moment description has led to more useful design and simulation tools, including a new version of BEDLAM[6]. The new BEDLAM code promises to be an efficient way to do 3-D problems involving space charge, without sacrificing accuracy or consuming huge amounts of computer time computing the 3-D effects.

SACHERER'S RESULTS

The original work of Sacherer[1] on the rms envelope equation was a second-order moment calculation, which corresponds to the effects of first-order (linear) forces. Let us redo his calculation using our present moment notation. For simplicity, we will do this for one degree of freedom. There are three second-order moment equations.

$$\begin{aligned} \frac{d}{dt}\langle x^2\rangle &= \frac{2}{m}\langle xp\rangle \\ \frac{d}{dt}\langle xp\rangle &= \frac{1}{m}\langle p^2\rangle + \langle xF\rangle \qquad (1) \\ \frac{d}{dt}\langle p^2\rangle &= 2\langle pF\rangle \end{aligned}$$

We can eliminate $\langle p^2\rangle$ in favor of ϵ_{rms}, the rms emittance, which is the following function of second moments

$$\epsilon_{rms} = \frac{1}{mc}(\langle x^2\rangle\langle p^2\rangle - \langle xp\rangle^2)^{1/2}. \qquad (2)$$

Assume the rms emittance is a known function of time. This reduces the number of equations from three to two:

$$\begin{aligned} \frac{d}{dt}\langle x^2\rangle &= \frac{2}{m}\langle xp\rangle \\ \frac{d}{dt}\langle xp\rangle &= \frac{\langle xp\rangle^2}{m\langle x^2\rangle} + \frac{mc^2\epsilon_{rms}^2}{\langle x^2\rangle} + \langle xF\rangle. \end{aligned} \qquad (3)$$

If we least-squares fit the force F to a linear function of x, $F = kx$, the force constant k turns out to be $\langle xF\rangle/\langle x^2\rangle$. Thus the last term in the second moment equation above can be written as $k\langle x^2\rangle$. Therefore, the evolution of the second moments depends only on the linear part of the force, determined by least-squares fitting.

Now assume that the force is composed of a linear external focusing force and an arbitrary space-charge force.

$$F = -k_{ext}x + F_{sc} \qquad (4)$$

Then the moment equations become

$$\begin{aligned} \frac{d}{dt}\langle x^2\rangle &= \frac{2}{m}\langle xp\rangle \\ \frac{d}{dt}\langle xp\rangle &= \frac{\langle xp\rangle^2}{m\langle x^2\rangle} - k_{ext}\langle x^2\rangle \\ &\quad + \frac{mc^2\epsilon_{rms}^2}{\langle x^2\rangle} + k_{sc}\langle x^2\rangle \end{aligned} \qquad (5)$$

where the space-charge force constant is given by

$$k_{sc} = \frac{\langle xF_{sc}\rangle}{\langle x^2\rangle}. \qquad (6)$$

Equation 5, which is a system of two first-order equations, is equivalent to the single second-order equation for the rms envelope given in Sacherer's paper. Sacherer has shown that the space-charge force constant k_{sc} is given by

$$k_{sc} = \frac{\text{const.}}{\langle x^2\rangle^{1/2}}, \qquad (7)$$

where the constant is almost independent of the shape of the charge distribution. He did this by computing the constant for uniform, parabolic, Gaussian, and hollow ($x^2\times$

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Gaussian) distributions. Thus we can use any convenient model to compute k_{sc}, without regard to the particular charge distribution under consideration.

THE TRACE3D CODE

The equations above assumed the rms emittance to be a known function of time; often we just assume it to be constant. This is a very reasonable assumption for the usual application of Sacherer's results, which is found in design codes like TRACE3D[3]. These codes are used to design beamlines. While emittance growth could in general be substantial, final designs, for which the beam is matched to the beamline, usually will not experience significant emittance growth and thus be accurately described by the Sacherer model.

Sacherer presented results also for three degrees of freedom[1]. For this situation, the rms emittances are not conserved, even for purely linear forces. The moment invariants, described below, are the conserved quantities. TRACE3D handles this situation correctly because it evolves the σ-matrix, which is a description in terms of the 21 second moments that exist for 3 degrees of freedom.

Since the space-charge force constant is nearly independent of the distribution details, we can use any "equivalent" beam to represent the actual beam. Here, "equivalent" means having the same second spatial moments. It would be convenient to take some simple equivalent beam for which we can solve the equations of motion and watch the behavior of its second moments, which should be close to those of the beam we are trying to simulate. But there is no beam that we know how to solve. If we assume a beam initially uniform in (x,y,z), then after one time step, it is no longer uniform. There is no such thing as a TRACE3D model distribution. What happens is that, at each time step, the space-charge force constant is computed from the second spatial moments, assuming a uniform charge density in a (x,y,z) ellipsoid. Though we do not assume that an initially uniform beam stays uniform and though we do not know what the distribution is like in detail, because of Sacherer's result we do not care[†].

Given our present knowledge, it appears that the physics of TRACE3D is as good as it can be for a linear-force (second moments) model. Unfortunately, there is no way to directly compare TRACE3D or other similar linear code with a particle simulation.

OTHER MOMENT RESULTS

The rms emittance is a function of second moments that is conserved in systems with linear forces having one degree of freedom. Recently, a whole family of functions of moments were discovered to be invariant for linear motion in systems with one, two, and three degrees of freedom[7, 8, 9, 10]. These moment invariants are conserved for linear motion, even in the presense of coupling. For example, the following is an invariant that is a function of second moments and is valid for two degrees of freedom.

$$\begin{aligned} I_{22} \;=\; & <x^2><p_x^2> - <xp_x>^2 \\ & + <y^2><p_y^2> - <yp_y>^2 \\ & + 2<xy><p_xp_y> - 2<xp_y><yp_x> \end{aligned} \qquad (8)$$

This is the sum of the squares of the rms emittances in the two directions plus a coupling term. There is another independent invariant that is a function of second moments. For three degrees of freedom, there are three invariants. There are also invariants that are functions of higher moments. For example, the following invariant is a quadratic function of fourth moments for one degree of freedom.

$$I_{44} = <x^4><p_x^4> - 4<x^3p_x><xp_x^3> + 3<x^2p_x^2>^2 \qquad (9)$$

The moment invariants can be used as diagnostics in simulation codes. This is done by computing the invariants at each time step and observing where they begin to change. Changes indicate the presence of nonlinear effects. Rms emittances are not useful indicators of nonlinear effects in systems with bends, for example, because the emittances can change from from longitudinal-transverse coupling as well. We observe rms emittance growth inside the bend. The emittances are restored to nearly their initial values at the end of the bend, if the bend is achromatic. The source of any unrecoverable emittance growth can be readily seen by examining where the growth of the moment invariant occurred. This technique has been applied to PARMILA simulations for beamlines containing skew bends in which the coordinate rotations introduce rms emittance growth that is not present at the end of the beamline[11]. There exists a simple algorithm for numerically computing the second-moment invariants[9], which is useful for such applications.

THE MOMENT CODE BEDLAM

The original BEDLAM code numerically integrated the moment equations, using a collection of initial moments as the initial conditions. This code suffered from an instability problem that prevented the simulation of systems more than a few focusing periods long. We could not use a symplectic integrator to achieve stability because the moment equations cannot be put into the form of Hamilton's equations. An important recent result was the discovery that the moment equations can be put into a Hamiltonian formulation[12] using a generalization of the Poisson-bracket formulation. This work led to the development of Lie-Poisson integrators[13, 14] that preserve the bracket structure exactly, achieving numerical stability analogous

[†]Appendix D of the TRACE3D manual discusses a 6-D distribution with ellipsoidal symmetry that is uniform in all 3-D projections. The rms emittances of this distribution are shown to be one-fifth of the total emittances. No such distribution exists. But this is not a problem as the existence of such a distribution is not used in any way by TRACE3D. All that matters is that $<x^2>$ is one-fifth of the maximum x^2 value for an ellipsoidal distribution uniform in (x,y,z). So we must scale all rms coordinates by $\sqrt{5}$ when presenting data to TRACE3D, which is what the manual instructs.

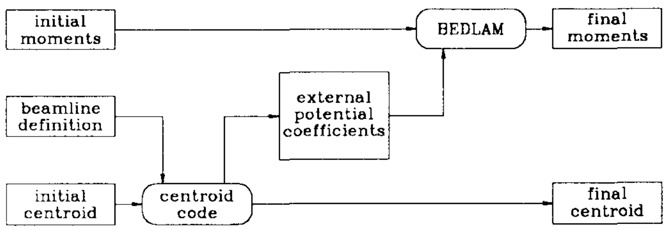

Fig. 1. Data flow at the top level for a BEDLAM simulation. Rectangular boxes indicate data files and boxes with rounded corners indicate processes that transform data.

to that provided by symplectic integration. The new BEDLAM code[6] uses Lie-Poisson integration. (Also, the new code has an improved space-charge model.)

Because of restrictions imposed by the Lie-Poisson integrator, the first moments (beam centroids) are handled separately in the new BEDLAM. Figure 1 shows the data flow for a BEDLAM simulation. We need a separate "centroid code" to compute the first moments and generate the external-force expansion used by the actual BEDLAM code. The centroid code provides the user interface. Various existing particle codes could be modified to be centroid codes for BEDLAM. Since the centroid motion is not affected by space charge (to good approximation) all we need of the centroid code is to trace a single particle, without space charge and evaluate the focusing forces at the centroid particle's location at each time step. BEDLAM will then do the difficult job of determining the high-order motion in the presence of 3-D space charge.

DISCUSSION

The moment approach is useful because moments are closely related to observable quantities and also simply because it deals with the distribution rather than the single-particle motion. Linear design codes are based on the moment work of Sacherer. New results are the discovery of moment invariants and the development of Lie-Poisson integrators. High-order moment codes are expected to provide accurate 3-D space-charge simulations. Furthermore, the efficiency of the moment method may mean we can have high-order design codes, using optimizers.

The new BEDLAM code is almost ready for testing on real problems. We will soon know if the promises of the new approach will be realized. There is work now in progress that promises even more improvements. Alternate Lie-Poisson integrators can handle more general Hamiltonians. A new scheme being investigated by P.J. Channell and J.C. Scovel should be able to handle the first moments directly in the moment code. Improved moment simulations could use moment invariants as the dynamical variables, thus factoring out the linear motion. By solving directly for the nonlinear effects, we should be able to improve numerical efficiency in a manner that action-angle or amplitude-phase methods do for single-particle motion.

The BEDLAM space-charge model contains nonlinearities to all orders that are truncated to the order appropriate to the order of the moments (linear forces for second-order moment simulations and cubic forces for fourth-order simulations). Therefore, a second-order BEDLAM simulation is not the same as a TRACE3D simulation. BEDLAM in its present form does not use Sacherer's idea of using least-squares fits to get the forces[‡]. Testing of BEDLAM will quantify how useful Sacherer's idea really is. The high-order analog of this scheme would be (for fourth-order BEDLAM) to do a least-squares fit to fit the space-charge forces to a cubic polynomial. Some related work has already been done[15]. One question to answer is: How much improvement would the least-squares fit bring? And can we do better simply by running BEDLAM to a higher order?

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‡In TRACE3D, the space-charge model (uniformly charged ellipsoid) corresponds to linear forces so the least-squares fit is the same as taking the linear part. In BEDLAM, the situation is not so simple.