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STATUS OF THE BEDLAM OPTICS CODE*

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ABSTRACT.

The BEDLAM simulation code (BEam Dynamics in Linear Accelerators by Moments) represents the beam by its phase-space moments. Here, we present a status report on our work in developing this approach, which is an efficient way to compute 3-D beam motion to high order. The space-charge algorithm, which extends Sacherer's results to higher order, now works well for some test cases but is inaccurate for others. We found that for high-brightness beams, higher-order motion is qualitatively different from that predicted by the linear model. While this means BEDLAM is modeling real-beam behavior not seen in the linear model, it makes it difficult to compare BEDLAM to linear codes. We have also verified the feasibility of using BEDLAM to do nonlinear matching.

INTRODUCTION

In the BEDLAM code,¹⁻³ we represent the beam by moments of its phase-space distribution. Moments are averages of monomials in the phase-space variables. For example, the moment $\langle x^2 \rangle$ is the average value of x^2 . At present, the BEDLAM code considers moments up to fourth order (force to third order). Given a set of initial moments, BEDLAM numerically integrates the moment-evolution equations using a Lie-Poisson integrator, which preserves the Hamiltonian structure. The integrator has proved to be stable as expected. The space-charge effects are computed using an extension of Sacherer's ideas to higher order. In this paper, we review these principles and present the results of recent tests of the space-charge model. We also compare BEDLAM to second-moment (linear force) codes like TRACE3D. There are fundamental differences in the dynamics because BEDLAM includes nonlinear forces. The final topic concerns nonlinear matching, a new capability made possible by the moment approach.

SIMULATION BY MOMENTS

There are at least three advantages to describing a beam by its moments. First, this description deals with distributions rather than with single-particle motion. This is important in studying matching. For example, if a beam is matched to a periodic focusing system, then all the moments are periodic. This is a much cleaner situation than in a particle description in which the individual particle motions contain betatron-frequency components that average to zero only when the whole distribution is considered. Second, the moments are closely related to laboratory quantities like beam sizes and divergences. Finally, using moments, the computational cost for 3-D simulations is little more than for 2-D simulations of the same accuracy. For example, for fourth-order simulations, the number of moments in 3-D is only about 4 times that in 2-D. In a mesh method (particle-in-cell code), the amount of work increases by the number of mesh points in the third direction, which could be considerable. For this reason, we believe the BEDLAM code will be useful in studying high order, 3-D space-charge effects in high-brightness beams.

The equation for the evolution of the $\langle xp_x \rangle$ moment is derived as follows.

$$\begin{aligned} \frac{d}{dt} \langle xp_x \rangle &= \left\langle x \left(\frac{d}{dt} p_x \right) \right\rangle + \left\langle p_x \left(\frac{d}{dt} x \right) \right\rangle \\ &= \frac{1}{m} \langle p_x^2 \rangle + \langle x F_x \rangle \end{aligned}$$

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Figure 1. Data flow for a BEDLAM simulation. The rounded boxes are processes that transform data.

$$\begin{aligned}
 &= \frac{1}{m} \langle p_x^2 \rangle + \langle x(a_0 + a_1 x + a_2 y + a_3 z + a_4 x^2 + a_5 xy + \dots) \rangle \\
 &= \frac{1}{m} \langle p_x^2 \rangle + a_0 \langle x \rangle + a_1 \langle x^2 \rangle + a_2 \langle xy \rangle + a_3 \langle xz \rangle + a_4 \langle x^3 \rangle + a_5 \langle x^2 y \rangle + \dots
 \end{aligned} \tag{1}$$

We have replaced the force F by a polynomial approximation. This turns the integral on the right side into a sum of moments. The other moment equations are similar. If we truncate the moments at some order, we get a system of ordinary differential equations for the moments. The present version of BEDLAM truncates after fourth order so there are 203 moments and a corresponding number of evolution equations for these moments. (BEDLAM treats the six first moments separately because of limitations imposed by our integrator.) BEDLAM numerically integrates the truncated system starting with a set of initial moments.

The moment-evolution equations are not in the form of Hamilton's equations (the moments cannot be paired into coordinates and conjugate momenta). This means we cannot use symplectic integrators to solve the differential equations. However, the moment equations do have a Lie-Poisson structure, which is related to the Poisson bracket. We have developed Lie-Poisson integrators⁴ that preserve this bracket structure exactly. This provides the numerical stability analogous to that provided by symplectic integrators for single-particle motion.

Figure 1 shows how a BEDLAM simulation works. The first moments (beam centroids) are treated separately. The inputs to the BEDLAM code itself are the 203 second through fourth initial moments and the external-potential-expansion coefficients, evaluated at the centroid positions. The BEDLAM code internally computes the space-charge effects from the beam moments. The output of bedlam is the vector of moments at the end of the time step.

SPACE-CHARGE ALGORITHM

At each time step in the simulation, we need to compute the 31 coefficients to a fourth-degree polynomial that approximates the space-charge potential.

$$U(\vec{r}) = u_1 x^2 + u_2 xy + u_3 xz + u_4 y^2 + \dots + u_{31} z^4 \tag{2}$$

These coefficients are computed from the 31 purely spatial moments that make up the 203 second through fourth moments. Our algorithm uses a generalization of Sacherer's results of 1971.⁵

Sacherer's Results

Sacherer's results, which relate to the evolution of the second moments, are

1. Moment evolution depends on the nine integrals $\langle x_i p_j \rangle$.

Figure 2. The curve shows a typical space-charge force as a function of distance x . The fitted linear force has a slope less than that of the actual force's slope at the origin.

2. These integrals are almost independent of distribution details (higher moments).

We have seen in Eq. 1 how the first result arises. The second result was obtained by computing the $\langle x_i F_j \rangle$ integrals for a variety of distributions having the same values of the second spatial moments ($\langle x_i x_j \rangle$). For the case of second moments, the space-charge force must be replaced by its linear approximation.

$$F_x = k_{fit} x, \quad (3)$$

where the fitted force constant k_{fit} is chosen by

$$k_{fit} \langle x^2 \rangle = \langle x F_x \rangle \quad (4)$$

Sacherer's second result says that we can use any convenient model to compute the integral $\langle x F_x \rangle$. Figure 2 shows a typical space-charge force field, which is linear near the origin and drops off as r^{-2} at infinity. Since the fitted force constant takes into account the whole beam, its value is less than the slope of the force field at the origin. Equation 4 is actually the condition that minimizes the least-squares error in $k_{fit} x - F_x$.

Extension of Sacherer's Results to Higher Order

In the case of fourth-order moments, the evolution is determined by 57 generalized Sacherer integrals, which are $\langle m_i F_j \rangle$, where the m_i are the 19 monomials of degrees one through three. Sacherer's second results holds when extended to higher order. Table I shows some of the values of the integrals $\langle x F_x \rangle$ and $\langle x^3 E_x \rangle$ for a spherically-symmetric beam with various radial charge distributions. All distributions have the same value of the second moment $\langle x^2 \rangle$. (The integrals are normalized to the uniform-beam case.) The values of $\langle x F_x \rangle$ for the first four distributions are the same as in Sacherer's paper. We see that this integral is nearly constant, regardless of the distribution. The surprising fact is that $\langle x^3 E_x \rangle$ is also nearly constant, even though we have not fixed the fourth moments. So we have even more than is required (that $\langle x F_x \rangle$ and $\langle x^3 E_x \rangle$ depend only on moments of order fourth and lower).

Table I. Sacherer integrals for various spherically-symmetric charge distributions. For the Gaussian and hollow distributions, there is a cutoff at 5σ . All distributions have the same second moments

distribution	$\langle x E_x \rangle$	$\langle x^3 E_x \rangle$
uniform	1.00	1.00
parabolic $1 - r^2$	1.01	1.02
Gaussian $e^{-r^2/2\sigma^2}$	1.05	1.03
hollow $r^2 \times e^{-r^2/2\sigma^2}$	1.02	1.02
r^4	1.02	0.96
r^8	1.04	0.94

We have developed an algorithm that determines the 31 space-charge potential coefficients of Eq. 2 from the 31 spatial moments. We can simplify the computation if we augment the vector of the 31 spatial moments with the fixed zeroth and first moments to form a 35-component vector of moments π_i . At each time step, the computation of the 31 space-charge potential coefficients U_i is given by a matrix multiply

$$U_i = T_{ij} \pi_j, \quad (5)$$

where T_{ij} is a 31×35 matrix. This matrix does not have to be recomputed at each time step but only after the beam has undergone a substantial change in size in any direction.

The matrix T_{ij} is derived in two steps. First, we compute the 35 charges in a charge model consisting of 35 Gaussian charges. These charges are chosen by making the spatial moments of the 35-Gaussian model match those of the beam being simulated. Now assuming this charge model, we obtain the 31 potential coefficients by requiring the field of the model to match the field of the polynomial approximation at N "evaluation points." If the evaluation points are distributed like the actual beam, then this procedure minimizes the error in the 57 generalized Sacherer integrals $\langle x_i F_j \rangle$, which determine the evolution of the moments. The 31 coefficients are passed to the integrator (after adding the external-forces part) and the integrator builds the Sacherer integrals.

TEST OF SPACE-CHARGE ALGORITHM

To test the space-charge algorithm, we considered a 3-D example we could compute analytically: a charge distribution consisting of two spherical Gaussians. To judge the accuracy of the algorithm, we compared the exact value of the following Sacherer integrals (which are the largest of the 57) to the BEDLAM result.

$$\begin{aligned} \langle x F_x \rangle \quad \langle y F_y \rangle \quad \langle z F_z \rangle \\ \langle x^3 F_x \rangle \quad \langle y^3 F_y \rangle \quad \langle z^3 F_z \rangle \end{aligned}$$

We used the BEDLAM values of u_i in

$$F_x = -\frac{\partial}{\partial x} [u_1 x^2 + \dots + u_{31} x^4] \quad (6)$$

to compute numerically the Sacherer integrals corresponding to the BEDLAM simulation. For our examples, we have 75% of the charge in one Gaussian and 25% in the other. Table II shows the results for various cases in which we varied the separation of the Gaussians and their widths (σ values).

Table II. Maximum of errors in the six Sacherer integrals for five cases of double Gaussian distributions

case	separation of centers	σ_1	σ_2	max error in Sacherer int.
1	1	0.5	0.5	2.6%
2	1	1	1	1
3	1	2	2	1
4	2.15	0.5	0.5	20
5	1	0.9	0.5	15

The **BEDLAM** calculations for Cases 1–3, which had equal widths for the two Gaussians, were very accurate. The Sacherer integrals, between cases, varied by more than a factor of three for the various widths but the algorithm computed them to within one or two percent. We also found that the results were not very sensitive to the overall size of the beam, which is evidence that the recalculation of the T_{ij} matrix of Eq. 5 would not have to be done often.

Case 4 also had equal widths but the separation of the Gaussians was large compared to the widths. This case was not accurately computed by **BEDLAM**, which is not surprising. This level of approximation (fourth order moments) is not good enough to model a charge distribution consisting of two separated blobs. Case 5 shows that we also get poor performance if the widths of the two Gaussians are different. This is an unexpected result. We plan further tests to understand the problem.

NONLINEAR SPACE-CHARGE DYNAMICS

TRACE3D is a second-order moment code (linear forces) that implements Sacherer's results by using a uniformly-charged ellipsoid space-charge model. To compare **TRACE3D** to **BEDLAM**, we simulated one period of a FODO channel of Halbach⁶ PMQs transporting a high-brightness beam. In our example, the tune depression was $\sigma/\sigma_o = 0.53$, which corresponds to a space-charge parameter value of $\mu = 1 - (\sigma/\sigma_o)^2 = 0.72$. We found poor agreement between the codes for this high-brightness beam, although the agreement was excellent with space charge turned off. We found poor agreement even when we truncated the **BEDLAM** force expansion to turn off nonlinearities.

Does this indicate a problem with **BEDLAM**? To see that it does not, consider the following. (For simplicity, we assume 1-D here, although both **TRACE3D** and **BEDLAM** are actually 3-D codes.) In **TRACE3D**, the space-charge force is linear

$$eE_x = k_{11}x, \quad (7)$$

where the space-charge force constant k_{11} is determined from the uniform-ellipsoid charge model using Eq. 4. In **BEDLAM**, we have a cubic force model

$$eE_x = k_{31}x + k_{32}x^2 + k_{33}x^3, \quad (8)$$

where the constants k_{31} , k_{32} , and k_{33} are chosen by

$$\begin{aligned} \langle x^2 \rangle k_{31} + \langle x^3 \rangle k_{32} + \langle x^4 \rangle k_{33} &= e \langle x E_x \rangle \\ \langle x^3 \rangle k_{31} + \langle x^4 \rangle k_{32} + \langle x^5 \rangle k_{33} &= e \langle x^2 E_x \rangle \\ \langle x^4 \rangle k_{31} + \langle x^5 \rangle k_{32} + \langle x^6 \rangle k_{33} &= e \langle x^3 E_x \rangle, \end{aligned} \quad (9)$$

which makes Eq. 8 a least squares fit to the actual force eE_x . The cubic model is, of course, a better approximation to the actual force than the linear model. This is illustrated schematically in the graph on the right in Fig. 3. The linear part of the cubic fit is larger than that for the linear fit, $k_{31} > k_{11}$. This difference can be a large effect.

When we want to characterize the strength of the space charge effect by a single number, we use the tune depression factor σ/σ_o or the space charge parameter μ . Let k_{eff} be the effective focusing force constant. For an alternating gradient focusing system, this means k_{eff} is the value of the time independent force constant that produces the same phase advance as the actual alternating gradient force. (This is often called the smooth approximation.) Then μ is given by

$$\mu = \frac{k_{eff}}{k_{eff} + k_{31}}, \quad (10)$$

where k_{eff} is the effective (smooth) space charge force constant, and can be the smooth equivalent of k_{11} , k_{31} , or the value of slope at the origin of the actual force. In 3-D, we can still describe

Figure 3. Left graph compares a Gaussian and a uniform charge distribution in 3-D. Both distributions have the same total charge and second moments ($\sigma = 1$) but very different central densities. The right graph shows that, for a typical distribution, BEDLAM's cubic-force model is more like the actual space-charge force than the linear model in TRACE3D.

the space-charge strength by a single number, even though there are three tune depressions, by using (smooth) potentials

$$\mu = - \frac{\nabla^2 \phi_{sc}}{\nabla^2 \phi_{ext}} \bigg|_0. \quad (11)$$

This means μ is proportional to the central charge density. Nonuniform beams can have much greater central charge densities than uniform beams having the same total charge and second moments. The left graph of Fig. 3 shows charge density ρ as a function of r for a uniform beam and a Gaussian beam with the same total charge and width ($x_{rms} = y_{rms} = z_{rms} = 1$). The graph is to scale. The central density of the Gaussian is about three times that of the uniform beam.

Thus we see that for a situation with a moderately high μ value in a linear code like TRACE3D, the μ value using the cubic model (or the actual space-charge force) can be greater than unity. This does make sense. Near the center of the beam the space charge force can be larger than the external focusing force. Even though μ is larger than unity, the motion can be stable, consistent with the smaller-than-unity value of μ given by the linear model, in which the whole beam is modeled by a different, smaller effective space-charge force constant. Figure 4 shows the phase-space trajectories for this situation. For small $|x|$, the motion looks unstable; the orbits are like hyperbolas. However, the overall motion is stable; the phase-space orbits circle the origin. We see that for bright beams, higher-order space-charge effects introduce qualitatively different behavior. We need to further study how well BEDLAM is modeling this new behavior.

MATCHING WITH BEDLAM

Fig. 5. Data flow for matching with BEDLAM. The BEDLAM code transports initial moments to their final values. The MATCHER code computes a suggested initial set of moments for BEDLAM to try. This process is repeated until the moments stop changing.

The moment approach makes it easy to do nonlinear matching. For a periodic channel, a matched beam has all moments periodic. We have tested the idea of computing matched beams by writing a matching code. This code is separate from the BEDLAM code. It reads the final moments computed by BEDLAM and generates a new file of input moments, which can be used by BEDLAM. (At the present time, the matcher code simply averages the input and output moments of the BEDLAM run to get

Figure 4. Motion in phase space for nonuniform beams like Gaussians when $\mu > 1$. Motion for small $|x|$ appears unstable (hyperbolas in phase space) even though overall motion is stable (circles origin of phase space).

the new input moments. Since this simple algorithm does converge, we did not attempt to develop a more sophisticated method.) Thus to compute a matched beam, we just execute BEDLAM and the matching code alternately until the moments stop changing. Figure 5 shows this process. This approach of using a separate code to do the matching is practical because the amount of data is small (203 numbers). For our example, we took a PMQ channel without space charge. To enhance nonlinear effects, we used short magnets (length=bore) with small bores (bore= $2 \times x_{rms}$). With the nonlinearity of the magnet fringe fields temporarily turned off, we computed the matched beam. For this matched beam, all 203 moments final moments were the same as the initial moments. The transverse Courant-Snyder parameters for this linearly-matched beam are shown in Table IV, where it is called Beam A.

Table IV. Courant-Snyder Parameters for Matching Study.

	A. Linear match.		B. Final beam using beam A as input.		C. Matched to nonlinearities.	
	α	β	α	β	α	β
x	-1.4161	1.3475	-1.1985	1.0949	-1.3818	1.2261
y	1.4464	1.3478	1.5204	1.2447	1.3822	1.2270

When we turned the fringe-field nonlinearities on and ran Beam A through the channel, the final beam was not the same as the initial beam. This final beam is shown in Table IV as Beam B. Besides not having a match anymore, we found that the rms emittances decreased by 2%. This is not surprising. A mismatched beam in a nonlinear system is not expected to preserve emittance. Next we rematched by running the matcher-BEDLAM iteration cycle several times. We found a new matched beam. (The input and output were again identical.) This beam is shown in Table IV as Beam C. The emittance was preserved for this matched-to-the-nonlinearity case. Thus nonlinear matching works as expected. It computes a beam matched to a nonlinear system by adjusting all moments up to fourth order. The matched beam, which differs from the one matched to the linear system, preserves emittance.

Beams matched to periodic systems preserve all moments. The familiar Courant-Snyder parameters are a complete description only for uncoupled second order moments. These parameters are obtained from the second moments as follows:

$$\alpha_x = -\frac{1}{2} \frac{d^2 x^2 / dt^2}{x^2 / dt^2}$$

$$\begin{aligned}\beta_x &= \langle x^2 \rangle / \epsilon_x \\ \epsilon_x &= (\langle x^2 \rangle \langle p_x^2 \rangle - \langle x p_x \rangle^2)^{1/2}\end{aligned}\tag{12}$$

DISCUSSION AND CONCLUSIONS

Our 3-D space-charge tests with the two-Gaussian charge distribution obtained excellent results for the cases with both Gaussian widths equal, over a wide range of widths. The accurate determination of all Sacherer integrals means that we have access to high-order effects of space charge. However, the cases with different widths produced poor results that we cannot yet explain. We need to understand this behavior before we can predict new phenomena with BEDLAM.

With nonlinear codes (moment order > 2), space-charge models must be nonuniform, just as real beams are. As we have seen, this introduces the possibility of having space-charge μ values larger than unity for beams of even moderate brightness. The reason this happens is the nonorthogonal nature of the potential expansion. The linear part of a linear fit is different from the linear part of a cubic fit, for example. This behavior makes it hard to compare a high-order code like BEDLAM to linear codes like TRACE3D. The effect is real, however. A bright beam does have motion near the spatial origin that looks unstable, so a μ value that is greater than unity is reasonable. The higher-order motion is qualitatively different from the linear motion.

Although Sacherer's results appear to still apply at higher orders, we need to further develop the theory. The convergence of the truncated moment-evolution equations can be tested independently, using other codes. We can do this by using moment invariants,⁷ which are certain functions of moments that are conserved for linear motion. For truncated moment systems (as in BEDLAM), some of these linear invariants are conserved for the general (nonlinear) case. (I call these invariants BEDLAM invariants.) We can test the validity of the convergence of the truncated moment equations, using even nonmoment codes, by seeing how well the BEDLAM invariants are conserved.

As expected, nonlinear matching has been verified as a new capability. Since the matcher code is separate from BEDLAM itself, we have a flexible system in which various tools can be used together without linking them all beforehand into one huge code. This capability is possible because of the small amount of data that has to be handled in the moment approach. It now appears that an optimizer, which runs as a process separate from BEDLAM, will also be feasible.

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