MOMENTS IN PARTICLE-IN-CELL SIMULATIONS*

M. M. Berz[†] and W. P. Lysenko, AT-6, MS H829
Los Alamos National Laboratory, Los Alamos, NM 87545 USA

Summary

The moment equations that form the basis of the BEDLAM simulation code can also be used as a check on Particle-In-Cell (PIC) simulations. Moments can be computed as sums over the macroparticles used in the PIC simulations. These moments should satisfy the moment equations if the simulation is valid. A check has been done to sixth order for two cases: the RFQRZP code, which simulated a radio-frequency quadrupole (RFQ) linac, and the BEAMTRACE code, which simulated the final focusing system in a heavy ion fusion facility. We observed how well the moment equations were satisfied for various values of the independent-variable step size and the number of macroparticles. Generally, we found that the PIC codes satisfied the moment equations very well. Because our modified PIC codes were able to compute moments that satisfied the correct moment equations, we were able to use our modified version of RFQRZP, which we called RFQMOM, to work on another problem. Every moment simulation code has to include some truncation approximation. The error of this approximation can be determined by RFQMOM before actually writing the moment code. As an example, we investigated the accuracy of the truncation approximation that is used in the BEDLAM code.

Introduction

To simulate a linac with the moment method,[1] we first specify the input beam as a collection of moments. The simulation code then integrates the moment equations, which govern the time evolution of the moments. No particles are traced in this approach. The BEDLAM code,[2] which is currently under development, is a fourth-order moment simulation code.

There is another interesting use for the moment equations. We can compute the moments from the particles in a PIC simulation code. These moments must satisfy the moment equations if the simulation is accurate. Therefore, we can use the moment equations as a check on PIC simulations, which is similar to keeping track of the energy in a simulation with a time-independent Hamiltonian. The advantage of the moment check is that a large number of moments (209 in fourth order) are available as checks and that these checks are available even in the absence of symmetries.

In this paper we present the results of moment equation checking in the RFQRZP code, which is the standard RFQ simulation code in the RFQLIB system,[3] and in the BEAMTRACE code.[4] We will demonstrate that the moment equations are well satisfied by these PIC codes. Because of this, we were able to study the validity of the truncation procedure that is used in BEDLAM.

The Moment Equations

Let $g(\vec{x}, \vec{v}, t)$ be a function of phase space and time. We define $\langle g \rangle$ as follows:

$$\langle g \rangle = \int d\vec{x} d\vec{v} \, g(\vec{x}, \vec{v}, t) \, f(\vec{x}, \vec{v}, t) \quad , \tag{1}$$

where $f(\vec{x}, \vec{v}, t)$ is the normalized distribution function in phase space. The distribution function f is assumed to satisfy Vlasov's equation

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \frac{\partial f}{\partial \vec{x}} + \frac{1}{m} (\vec{F} + q\vec{E}) \cdot \frac{\partial f}{\partial \vec{v}} = 0 \quad , \tag{2}$$

where $\vec{F}$ is the external focusing force and $\vec{E}$ is the space-charge electrostatic field.

The dynamical variables in the BEDLAM code are the moments

$$\langle x_1^{n_1} \, x_2^{n_2} \, x_3^{n_3} \, v_1^{n_4} \, v_2^{n_5} \, v_3^{n_6} \rangle \quad .$$

The sum $n_1 + n_2 + \ldots n_6$ is the order of the moment. The time evolution of these moments is given by the moment equations:

$$\frac{d}{dt} \langle x_1^{n_1} \, x_2^{n_2} \, x_3^{n_3} \, v_1^{n_4} \, v_2^{n_5} \, v_3^{n_6} \rangle$$

$$= n_1 \langle x_1^{n_1-1} \, x_2^{n_2} \, x_3^{n_3} \, v_1^{n_4+1} \, v_2^{n_5} \, v_3^{n_6} \rangle$$

$$+ n_2 \langle x_1^{n_1} \, x_2^{n_2-1} \, x_3^{n_3} \, v_1^{n_4} \, v_2^{n_5+1} \, v_3^{n_6} \rangle$$

$$+ n_3 \langle x_1^{n_1} \, x_2^{n_2} \, x_3^{n_3-1} \, v_1^{n_4} \, v_2^{n_5} \, v_3^{n_6+1} \rangle \tag{3}$$

$$+ n_4 \langle x_1^{n_1} \, x_2^{n_2} \, x_3^{n_3} \, v_1^{n_4-1} \, v_2^{n_5} \, v_3^{n_6} a_1 \rangle$$

$$+ n_5 \langle x_1^{n_1} \, x_2^{n_2} \, x_3^{n_3} \, v_1^{n_4} \, v_2^{n_5-1} \, v_3^{n_6} a_2 \rangle$$

$$+ n_6 \langle x_1^{n_1} \, x_2^{n_2} \, x_3^{n_3} \, v_1^{n_4} \, v_2^{n_5} \, v_3^{n_6-1} a_3 \rangle$$

Here the following abbreviation has been used:

$$a_i = \frac{1}{m} (\vec{F} + q\vec{E})_i \quad . \tag{4}$$

Equation (3) is a set of coupled, first-order differential equations. Expanding the terms a_i in power series of x_i makes it possible to rewrite the last three terms of Eq. (3) in terms of moments. For details about the computation of the coefficients of the Taylor's series see Ref. 1. If the forces have non-linear terms, the computation of the temporal derivative of a moment of order n requires the knowledge of moments of orders $n+1$ and higher.

The Codes RFQRZP and BEAMTRACE

RFQRZP is a 3-D PIC simulation code contained in the RFQLIB system. It computes space-charge effects

using a 2-D r-z Poisson solver. The boundary conditions consist of a conducting circular cylinder and periodicity in the z-direction with period βλ. The equations of motion are integrated by means of a first-order, explicit, symplectic integrator.

For our example, we simulated the accelerator test stand (ATS) RFQ linac at Los Alamos.[5] This machine accelerates a 100-mA H⁻ beam with a normalized transverse emittance of 0.2 mm·mrad from 100 keV to 2 MeV. The space-charge effects in this machine are significant. The tunes for particles with small amplitudes are depressed by factors of approximately 0.5.

BEAMTRACE is a PIC code designed for the simulation of ion optical systems. It can include electric and magnetic multipoles, homogeneous and inhomogeneous electric and magnetic bending fields, and fringing fields. The numerical integration is done with a Runge-Kutta method of fourth order. The calculation of the space-charge forces is done with a Green's function method, which does not require the differentiation of a potential; however, this method cannot account for wall interactions.

For our BEAMTRACE example, we used a final focusing system in a heavy ion fusion facility.[6] The beam consists of ^{209}Bi at an energy of 10 GeV, a current of 1250 A, and a transverse phase space of $xy\alpha\beta$ = 5.6 · 3.6 · 22 · 34 cm²mrad². The focusing is achieved by a pair of two quadrupole triplets, which have two opposite bending fields in between them to provide shielding of the beamline against neutron radiation.

Computing Moments in the PIC Codes

Modified versions of the PIC codes were developed to compute moments at each time step. In addition to the moments of the distribution, we also computed the moments on the right-hand side of the moment equations that involve forces. Figure 1 shows the moments <xx> and <yy> for the Los Alamos ATS RFQ. These moments are the squares of the rms beam sizes in the x- and y-directions, respectively. The fast oscillations in these plots are related to the rf frequency, whereas the slow modulations are oscillations at twice the tune-depressed betatron frequency. The fact that the distribution (and therefore any of its moments) contains the betatron frequency means that the beam is not exactly matched. Figure 2 shows the moment
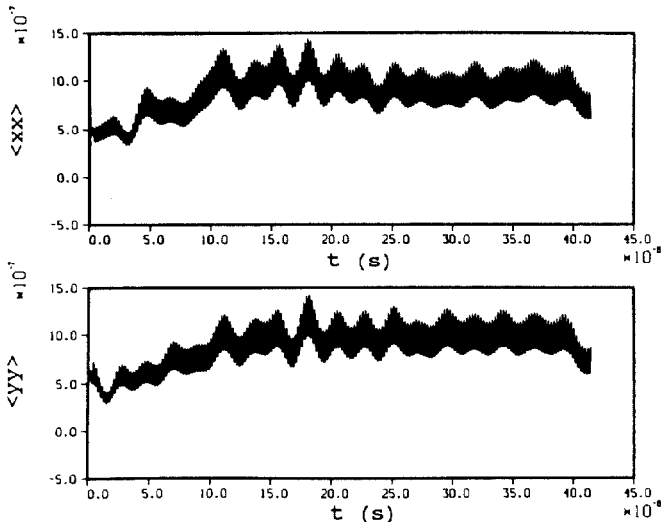

Fig. 1. The <xx> moment (top) and the <yy> moment (bottom) in the Los Alamos ATS RFQ (computed by RFQRZP).
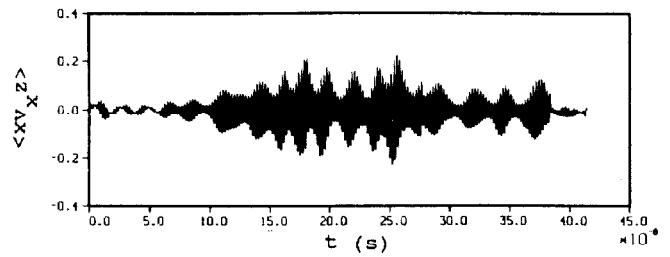
Fig. 2. The moment <xv_xz> in the ATS RFQ (computed by RFQRZP).

<xv_xz>, which is proportional to the correlation between the tilt of the ellipse in the x-v_x phase-space projection and the z-coordinate. Figure 3 shows plots of the moments <xx> and <yy> for the final focusing system of the heavy ion fusion facility, which were computed by BEAMTRACE.
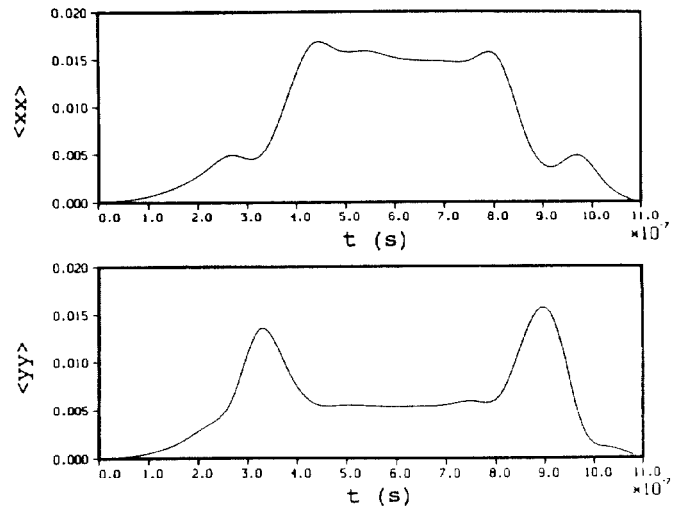
Fig. 3. The moments <xx> (top) and <yy> (bottom) for the final focusing system of the heavy ion fusion facility (computed by BEAMTRACE).

PIC Simulation Check Using the Moment Equations

After the modified PIC code has completed a simulation, the moments it has saved at every time step are analyzed by the CHECK program. CHECK numerically differentiates the moments using a five-point formula. It also computes the right-hand sides of the moment equations by adding up the appropriate moments. Then the error, by which we mean the relative difference between the left- and right-hand sides of the moment equation, is computed for each moment equation. We checked the moment equations for various time-step sizes. Generally, the error was larger for the higher order moments and for the larger step sizes. These results are practically independent of the number of macroparticles. (We tried from 50 to 5000 particles; the examples shown below used 1000 particles.) The minimum error we observed was about 10^{-3} for both the RFQRZP and the BEAMTRACE codes. Thus, both codes satisfy the moment equations, which are very general conditions not explicitly satisfied by the algorithms used. This serves as a significant test for the codes.

Figure 4 plots the RFQRZP simulation error, averaged over all moments of the given order, as a

function of the number of integration steps per rf period. The top curve is the error for moments of first order. (The first-order moments would all be zero in an ideal simulation. Their small magnitude gives rise to large relative errors in the first-order moment equations.) The other five curves in the graph are the errors for equations of orders two through six. Higher order moments have larger errors.
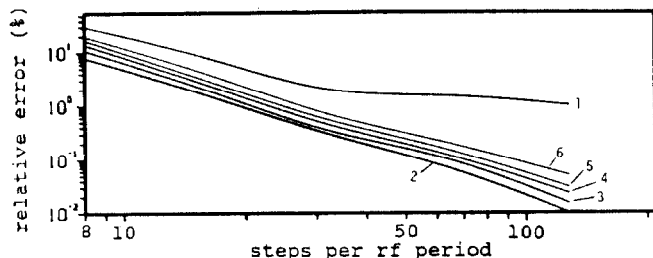

Fig. 4. The error in the moment equations for the RFQRZP simulation, averaged over all moments of the given order, as a function of steps per rf period. Each curve is labeled with the order of the moment equation to which it corresponds.

Moment Simulation Codes

We have seen that the particle simulation codes satisfy the moment equations quite well. Because the PIC codes could compute the moments accurately, we were able to use them to study the behavior of moment simulation codes. This way we can determine some of the characteristics of the moment codes even before they are written.

The moment equations are not closed. In the presence of nonlinear forces, the computation of the temporal derivative of order n requires moments of order n+1 and higher. To solve the moment equations, we must determine such higher order moments in terms of the lower order moments. There is no unique way to approximate the higher order moments. BEDLAM makes the approximation that higher order correlations are absent, which means that the higher order moments are written as products of lower order moments. The formula used is exact for Gaussian distributions.

We used the analysis program CHECK to compute the fifth- and sixth-order moments from the particle distribution. We also computed these moments from the lower order moments according to the approximation used in BEDLAM. We found that the average relative error in the higher order moments was more than 100% for the example of the ATS RFQ--it is probably just as accurate to neglect the higher order moments in the moment code simulations. Thus, the computation of the highest order moments (fourth order in BEDLAM) can take into account only linear force effects.

Although the higher order moments are poorly approximated, the right-hand sides of the moment equations are not necessarily highly inaccurate. Only some of the equations include the higher order terms that need approximation. For the low-order moment equations, the force expansion can be carried to a high order, probably including most of the nonlinear effects. But even the highest order moment equations

include at least the linear part of the force, which is usually the predominant part. Using the CHECK analysis code we determined the error in the right-hand sides of the moment equations arising from the approximation of the fifth- and sixth-order moments. The second-order moment equations had right-hand-side errors of about 1% on average. The other equations had right-hand-side errors of between 2 and 10%.

Conclusion

Our investigation showed that the PIC codes RFQRZP and BEAMTRACE satisfy the moment equations very well. Because other PIC codes use quite similar algorithms, we do not expect that other PIC codes will significantly violate the moment equations. These checks were done to sixth order, and our examples included space-charge forces.

Because the moment equations were well satisfied by our particle codes, we can use these particle codes to analyze the behavior of moment simulation codes like BEDLAM. We were able to determine the accuracy of the approximation used in BEDLAM, which was required because the moment equations are not closed. We found that the approximation of higher order moments in terms of lower order moments was inaccurate. Setting the higher order moments to zero is probably just as accurate. Because of the inaccurate terms, the right-hand sides of the moments equations had errors of between 1 and 10%. This result is inconclusive. We cannot say whether or not the BEDLAM results will be accurate. If we determine a better approximation to the moments than is now in BEDLAM, this problem will certainly be eliminated. If we cannot find a better approximation to the higher moments, and if the errors in the moment equations cannot be tolerated, then we will have to take our moment equations to higher order to get good results. How high an order is required depends on how nonlinear the forces are because it is the nonlinearities that couple the higher moments to the lower moments.

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