A TEST SUITE OF SPACE-CHARGE PROBLEMS FOR CODE BENCHMARKING *†

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Abstract

A set of problems is presented for benchmarking beam dynamics codes with space charge. The test suite contains problems whose solutions can be found analytically or to very high accuracy using numerical methods. Simulation results are presented for problems in the test suite obtained using the MaryLie/IMPACT, Synergia, and MAD9P codes.

INTRODUCTION

In recent years large-scale simulation has become increasingly important, used in combination with theory and experiment, to study and improve the performance of existing accelerators, and to further our understanding of the physics of intense charged particle beams. A key issue for such simulations is the treatment of space-charge effects, which strongly influence the accuracy of the simulations. The requirements for parameters such as the number of macroparticles, the grid size, and the particle-advance step size depend on issues such as the beam intensity and the path length of the simulated beam. The path length, in particular, can vary from roughly a kilometer in a linac or cyclotron, to thousands of kilometers in a booster or accumulator ring, to millions of kilometers in a large synchrotron. Long-term simulations of beams with space charge in circular accelerators represents one of the most challenging problems in computational accelerator physics.

In order to have confidence in our space-charge simulations, and to choose simulation parameters that provide the desired accuracy for the particular problem at hand, we have begun to assemble a test suite of space-charge problems for code benchmarking. The suite presently contains problems for which the solutions are known either analytically or are can be found to essentially arbitrary accuracy through numerical means. Other benchmarking efforts are also underway, some of which involve a comparison of simulated results with experiments. See, for example [1], which is based on experiments at the CERN-PS.

THE TEST SUITE

KV Beam in a FODO Channel

This test problem consists launching a matched KV distribution in a FODO channel. The beam and transport system parameters are as follows:

```
beam, particle=proton, ekinetic=6.7d-3 &
    bfreq=10221.05558d6, bcurr=0.50d0
drs: drift, l=7.44d-2
drl: drift, l=14.88d-2
qd7: quadrupole, l=6.10d-2, g1=-38.64d0
qf7: quadrupole, l=6.10d-2, g1= 38.64d0
cell, line=(drs qd7 drl qf7 drs)
```

The above specifies a 0.5 Amp, 6.7 MeV proton beam. The quadrupole strength is specified by g1 (instead of the usual k1) in T/m. The beam definition and lattice description, along with an initial distribution of macroparticles, are all that is needed to perform the simulation. For completeness, we list the following additional information: The unnormalized rms emittances are given by $\epsilon_x = \epsilon_y = 1 \times 10^{-6}$m-rad. The matched rms parameters at 0.5 amp are $x_{rms} = y_{rms} = 0.859 \times 10^{-3}$m, $p_{x,rms} = p_{y,rms} = 3.10 \times 10^{-3}$, $(xp_x)_{rms}/(x_{rms}p_{x,rms}) = -0.927$, $(yp_y)_{rms}/(y_{rms}p_{y,rms}) = 0.927$.

Since this is a 2D test problem, the space-charge calculation is performed by applying periodic boundary conditions in the longitudinal coordinate, z. The length of the computational box in the beam frame is $\gamma\beta c/b_{freq}$, where b_{freq} is equal to bfreq. (This, however, is not part of the benchmark specification; it is a parameter selected by the user, similar to the number of grid points, number of space-charge kicks, etc.) Figure 1 shows the output from two codes, Synergia and MaryLie/IMPACT (ML/I), which have been developed under a U.S. DOE SciDAC project [2]. The initial distribution contained 100,000 particles, adjusted to have the exact initial second moments of the matched beam. The space-charge calculation was performed using a 64x64x128 grid with open boundary conditions. In this case both codes give nearly identical answers (to within about 0.25%). This slight variation in the final answer is due to minor differences in the implementation of the Poisson solver [3] and differences in the number of slices used in the split-operator particle advance algorithm. For this test problem, numerical inaccuracies manifest themselves, for example, by rms mismatch and rms emittance growth. We verified that with increasing number of macroparticles and mesh points, the numerical emittance growth and mismatch were reduced.
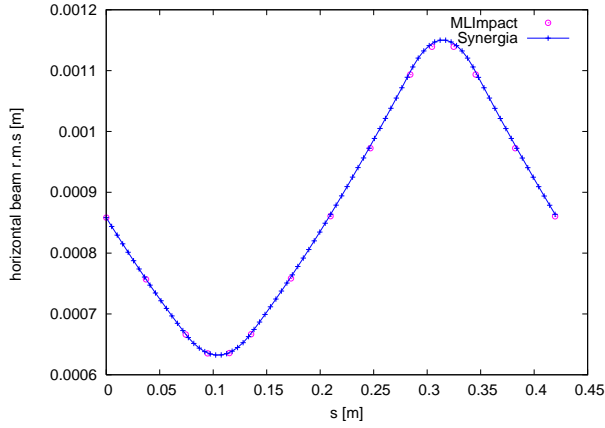
Figure 1: ML/I and Synergia results showing the rms beam size of a matched beam in a FODO channel

Free Expansion of a Cold Uniform Density Bunch

For this test problem, we model a cold, uniform density, proton beam with $\gamma = 2$ expanding in free space. This test case consists of two problems: (1) a spherical beam with radius 2 cm, and (2) an ellipsoidal beam with semi-axes $1.5 \times 2.5 \times 4.5$ cm. As an example, Figure 2 shows the output for the ellipsoildal case produced by a code based on MAD9P enhanced with three Poisson solvers: a particle-particle solver, a particle-mesh solver, and a hierarchical tree solver. The figure shows the fractional change of the horizontal rms beam size from the solution computed from the 3D envelope equations.
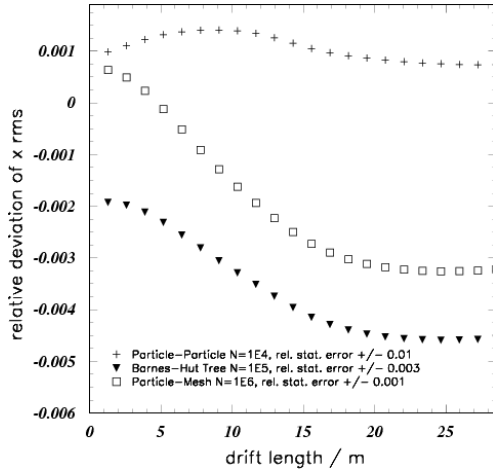

Figure 2: Simulation results using three different Poisson solvers showing the deviation in horizontal beam size from the exact solution for a cold ellipsoidal beam expanding in free space.

Cold Beam in a FODO Channel with RF Cavities

This problem involves a cold, uniform density, 250 MeV, 100 mA proton beam in a lattice described as follows:

```
beam, particle=proton, ekinetic=250.d-3 &
      bfreq=700.d6, bcurr=0.1d0
dr: drift, l=0.10  slices=4
fquad: quadrupole, l=0.15  g1=6.00  lfrn=0. &
           tfrn=0.  slices=6
dquad: quadrupole, l=0.30 g1=-6.00  lfrn=0. &
           tfrn=0.  slices=12
gapa1: rfgap,freq=7.e8,escale=40.e6, &
           phasedeg=45.,steps=100,slices=5
gapb1: rfgap,freq=7.e8,escale=40.e6, &
           phasedeg=-1,steps=100,slices=5
cell, line= &
  (fquad dr gapa1 dr dquad dr gapb1 dr fquad)
```

For 3D bunched beam problems, the charge per bunch is equal to `bcurr/bfreq`. In addition to the usual MAD beamline elements, a new element, rfgap, is shown above. It describes an rf cavity for which the on-axis field is given by $E(z) = E_0 \cos(\omega t + \phi)$. Values of the quantity $E(z)$ are stored in a table. In the above, `phideg` corresponds to the absolute phase ϕ and `escale` corresponds to E_0. For this test problem, the tabulated values are of the function $E(z) = \exp(-4x^4)\cos(\frac{5\pi}{2}\tanh(5x))$. The cavity frequency is $700MHz$. For the test problem, due to the fact that the beam is cold, the rms equations describe the problem *exacly* so long as the beam remains cold and uniform. The cavity phases have been set so that the first cavity accelerates the beam and the second cavity decelerates it by the same amount. As a result, there is a matched condition where the final envelopes (as well as the energy) are identical to the initial values. We used a 3D envelope matching code to find the 3D matched beam parameters, and we generated a numerical realization of the matched uniform distribution. Any deviation from periodicity in the numerical simulations is purely numerical. We have modeled this system using the ML/I code. The matched rms envelopes obtained from the 3D RMS envelope equations, along with the ML/I results, are shown in Figure 2.
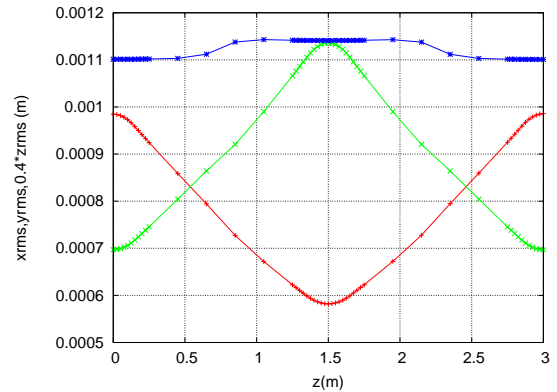

Figure 3: Plot of x_{rms} (red), y_{rms} (green), and t_{rms} (blue, scaled by 0.4 for plotting) versus distance in 1 period of a FODO channel with RF cavities. ML/I results (symbols) are on top of curves obtained from the RMS equations.

Thermal Beam in a Constant Focusing Channel

For this problem we model a stationary solution of the Vlasov/Poisson equations with spherical symmetry (cylindrical symmetry in the 2D case). For a stationary beam in a constant focusing channel, the Hamiltonian, H, is a constant of motion. In this case we choose a thermal distribution, i.e. $f(\vec{x}, \vec{p}) = C \exp(-H/kT)$, where C and kT are constants. Due to symmetry, the Poisson equation can be expressed as an ordinary differential equation for the scalar potential (suitably normalized), $\hat{\psi}$, as a function of r,

$$\frac{d^2\hat{\psi}}{dr^2} + \frac{2}{r}\frac{d\hat{\psi}}{dr} = -\exp(\frac{1}{2kT}(\alpha^2 r^2 + KC\hat{\psi})), \quad (1)$$

where α describes the external focusing strength, K is the perveance, and C is a constant that depends on the beam current. (Note that $2/r$ is replaced by $1/r$ in the 2D case). This equation can be solved to extremely high precision using numerical integration. The equation is integrated until the quantity $\frac{1}{r^2}\frac{d\hat{\psi}}{dr}$ (or $\frac{1}{r}\frac{d\hat{\psi}}{dr}$ in the 2D case) approaches a constant, which indicates that the electric field has reached its asymptotic free space value. This procedure results into a set of numerical values for $\psi(r)$, and hence the density $\rho(r)$, which can be tabulated and used to produce a sample representation of the stationary distribution. Because the distribution is stationary, any change in quantities such as second moments, rms emittances, and density profile are due to numerical errors. The 3D test case involves a proton beam of kinetic energy 0.1 MeV, external focusing strength of 2π rad/m, $kT = 36 \times 10^{-6}$, and current $I = 100$ mA.

Bi-thermal Beam, Constant Focusing Channel

A key feature in the previous example is that, due to symmetry, the Poisson equation was reduced to an ordinary (not partial) differential equation, which could be solved to extremely high accuracy in order to provide an "exact" solution . Unfortunately, the previous example exhibits very "simple" charge densities (varying from Gaussian at zero current to almost uniform in the extreme space-charge limit). This is not ideal for benchmarking, because often particle simulations are used to study beam halos. It is therefore very desirable to have a benchmark that exhibits a pronounced halo. This can be accomplished using an almost identical technique, except that we (self-consistently) superpose two distributions with different temperatures. In other words, the beam distribution function is taken to be a spherically symmetric distribution of the form $f(\vec{x}, \vec{p}) = C_1 \exp(-H/kT_1) + C_2 \exp(-H/kT_2)$, where C_1, C_2, kT_1, and kT_2 are constants. If we solve for the scalar potential of the first beam by viewing the second beam as providing an "external" field, and vice-versa, the result is that the problem is reduced to solving two coupled ordinary differential equations, one for ψ_1 and the other for ψ_2. For the test problem we model a 0.1 MeV proton beam with $kT_1 = 36 \times 10^{-6}$, $kT_2 = 900 \times 10^{-6}$, $I_1 = 99$ mA, $I_2 = 1$ mA. Figure 3 shows a plot of the exact density along with simulated density after 10 focusing lengths.
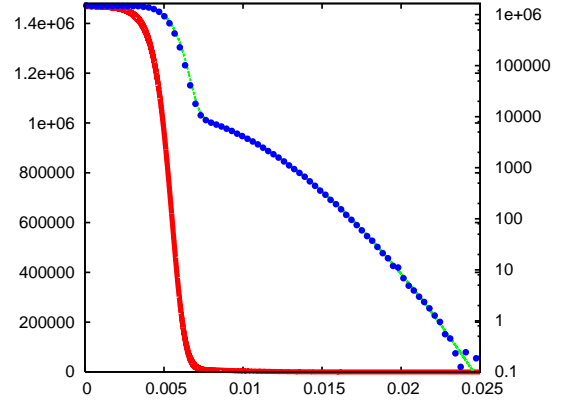

Figure 4: Beam density versus radius for a stationary, high-intensity bi-thermal distribution. The data are plotted on a linear scale (left axis, inner curve) and log scale (right axis, outer curve). The solid lines show the analytical solution as described in the text. The data points (circles, log scale) show the distribution after 10 focusing lengths, simulated using ML/I with 100 million particles. The halo is well-resolved out to a distance where the radial density is one million times smaller than the central density.

FUTURE DIRECTIONS

We have presented several examples that represent a starting point for a suite of problems to test and benchmark space-charge simulation codes. Web sites are being set up to contain the lattice descriptions and particle data sets so that users around the world can run identical problems and compare results. Because the data sets are large, two identical sites are being set up, one to be maintained by NERSC in the USA and one to be maintained by PSI in Europe.

So far we have made comparisons of quantities such as rms beam size and rms emittance. In the future we intend to make precision comparisons using quantities such as the 99.99% values of 2nd moments, which are much more demanding than rms quantities. Also, it would be very useful to have a test problem that includes not only a halo, but also a slow variation in parameters [4]; this would be the case, for example, for a beam undergoing slow synchrotron oscillations. It is unlikely that such a test case will be found for which the solution can be obtained analytically or seminumerically. Instead, such a problem will likely be solved using very high resolution particle simulation, and that will form the basis of another test case in the suite of codes.

REFERENCES

[1] http://www-wnt.gsi.de/ihofmann/Benchmarking/Benchmarking.htm

[2] See http://www.osti.gov/scidac/

[3] Both codes use a convolution-based algorithm for treating open systems as described, for example, in Hockney and Eastwood, "Computer Simulation using Particles."

[4] I. Hofmann, private communication.