

Quiet Start and Autotasking for PARMELA

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Abstract

The simulation code PARMELA has been widely used in the accelerator community for many years. Because of its simplicity, it is still used in many laboratories. When used to simulate the space charge in high current density electron bunches however, the results for the emittance and the other beam parameters can differ considerably from those obtained with PIC codes. This discrepancy comes in part from the noise introduced by the point to point space charge calculation used in PARMELA, when the particle distribution is not uniform. Here we present a new loading scheme which makes the initial distribution in the phase spaces more uniform and reduces greatly the noise introduced by artificial local bunching. At the same time, the code has been slightly modified in order to permit autotasking and vectorization on CRAY computers; the speed up factor obtained for the calculation time is proportional to 4 times the number of CPU available on the computer. Preliminary simulations of a 17 GHz RF Gun with the PIC code MAGIC and PARMELA show relatively good agreement considering that PARMELA does not handle Wakefields and radiations.

I. INTRODUCTION

In PARMELA, the space charge can be modeled by a point to point calculation: each particle is assigned a super charge and the Coulomb interaction between the particles is evaluated at each time step. When the number of particles in the simulation is large enough, this method gives relatively accurate results; however, because the CPU time scales as the square of the number of particles, it very quickly becomes prohibitive to use more than a few thousand particles. If the initial distribution for the particles is not uniform, artificial local bunching can appear, leading to high charge density areas which are not physical; this phenomenon is enhanced when the charge per macroparticle is increased, or when the number of particles in the simulation, for a constant total charge, is decreased. In Section II of this paper, a new loading scheme,

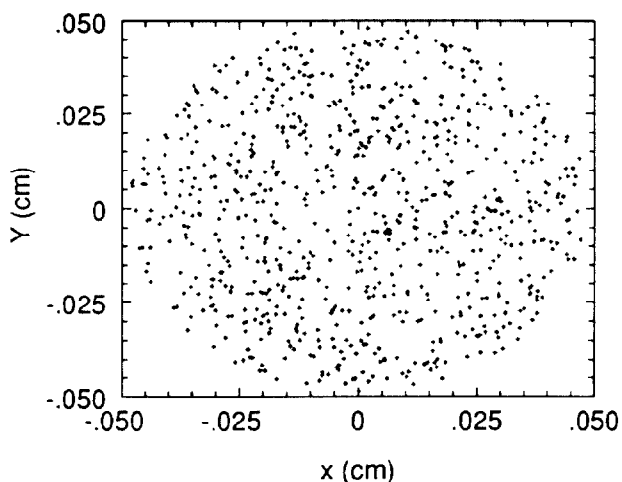


Figure 1: 787 particles sampled randomly in the transverse space.

successfully tested in FEL simulations, which greatly reduces this local bunching is described. Using this scheme, the calculated emittance is far less dependant on the number of particles in the simulation. In Section III, we briefly describe the modification of the source code in order to allow vectorization and autotasking. Finally, Section IV presents a preliminary comparison between the Particle in Cell code MAGIC, and this new version of PARMELA.

II. QUIET START

Figure 1 shows a typical distribution of the particles on the photocathode area of the 17 GHz Photocathode RF Gun being constructed at MIT [1]. The particles are sampled using the standard Fortran random number generator. It is easy to see "holes" and "bunches" due to the limited number of particles generated. As mentioned earlier this artificial local bunching leads to an increase in emittance which is not real. Figure 2

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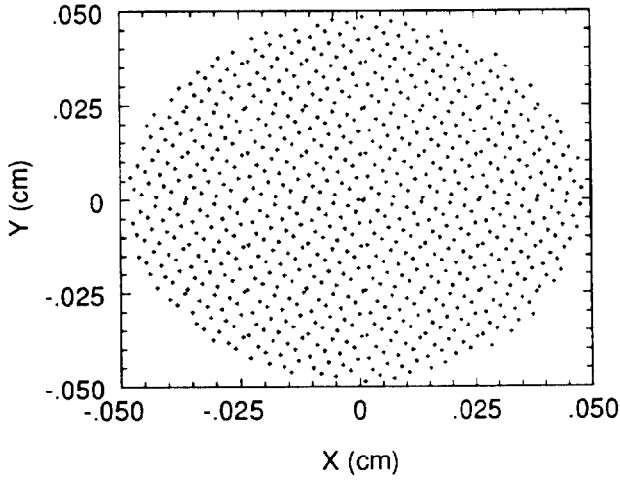


Figure 2: 787 particles sampled in the transverse space using Hammersley's sequence. x is sampled with $r=1$ and y with $r=2$

shows the same distribution sampled using the Hammersley's sequence [2]. Although there still are a few closely spaced points, the particles are evenly distributed in the transverse space. The Hammersley's sequence is defined as follows:

$$\{(j - \frac{1}{2})/N, \Phi_2(j), \Phi_3(j), \Phi_5(j), \dots, \Phi_r(j), \dots\}, \quad j = 1, \dots, N$$

where $\Phi_r(j)$ is the radial inversion function in the base of a prime number r :

$$\Phi_r(j) = a_0 r^{-1} + a_1 r^{-2} + \dots, \quad j = a_0 + a_1 r^1 + \dots$$

This yields for $r=2$ and $r=3$: $\Phi_2(j) = 1/2, 1/4, 3/4, 1/8, \dots$, $\Phi_3(j) = 1/3, 2/3, 1/9, 1/3 + 1/9, \dots$

A set of simulations for a 17 GHz photocathode RF Gun cavity was done using the two types of distribution (random and quiet start) and varying the number of particles simulated. Figure 3 shows that the emittance calculated using the Quiet Start (Hammersley's sequence) is lower and much less dependant on the number of particles than the one calculated using the random start.

III. AUTOTASKING AND VECTORIZATION

When the number of particles in the simulation is more than a few hundred, most of the calculation time is spent in the subroutine used to simulate the space charge effects. This subroutine is composed of two nested loops performing the point to point calculation. By making minor modifications inside the inner loop, and using the Fortran preprocessors available on

Emittance as a function of the number of particles

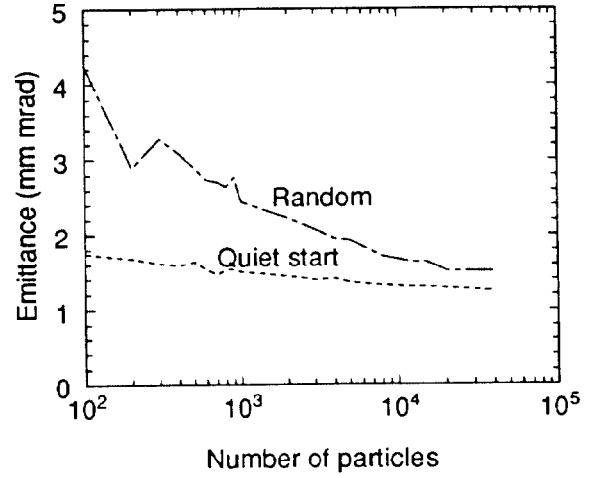


Figure 3: Emittance calculated using random and quiet start.

the CRAY computers [3] [4], the inner loop was vectorized and the outermost loop was parallelized. It should be noted however, that the calculation of the effect of the image charge in the cathode plane had to be eliminated. Work will be done in the future to reimplement this important effect. The speed up factor with only one CPU is 4 due to the vectorization of the inner loop. When using multi-CPU computers, the outermost loop is distributed among the different CPUs and the wall-clock time goes theoretically like the inverse of the number of CPUs. However, because the code is not 100 % parallel and because of the overhead produced by Autotasking, typical speed up factors of up to 10 for the wall-clock time on the 16 Processor CRAY YMP C90 have been observed. The extreme runs shown on Figure 3 correspond to 40000 particles and 113 time steps, corresponding to 12 hours of CPU time with one CPU.

IV. COMPARISONS WITH MAGIC

The 17 GHz photocathode RF Gun cavity being constructed at MIT has been simulated using the PIC code MAGIC and PARMELA. The fields calculated by MAGIC have been implemented in PARMELA in order to account for non linear RF effects. Figures 4 to 6 show the beam parameters at the exit of the cavity as a function of the charge, calculated by the two programs. The number of particles in the simulation in PARMELA is 500 and the effect of image charge in the cathode plane is included. The cathode radius is 0.5 mm, the laser pulse length 1.4 ps, and the initial phase is 12 degrees. The results for the radius and the divergence agree to within 10 % and those for the emittance and the bunch length agree to within 30 %. The situation is less favorable for the energy spread where the results can differ by a factor of 2 at low

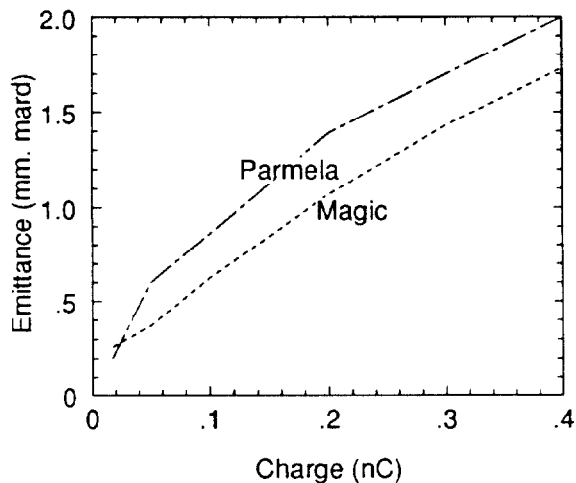


Figure 4: Emittance at exit of RF Gun cavity.

charge. The reason for this discrepancy is still under investigation.

V. CONCLUSIONS

A new loading scheme (Quiet Start) has been implemented in PARMELA; it makes the distribution of the particles in the transverse space more uniform and consequently reduces the noise level introduced by local bunching. The emittance is then much less dependant on the number of particles in the simulation. The point to point calculation subroutine has been parallelized and vectorized, leading to speed up factors of 4 in CPU time and potentially reducing the wall-clock time by a factor roughly proportional to the number of available CPUs on the computer. Preliminary comparisons with the PIC code MAGIC show an agreement to within 30 % for the emittance. However, it is not yet understood why the energy spread can differ by as much as a factor of 2 between the two codes. The reasons for this discrepancy are still under investigation.

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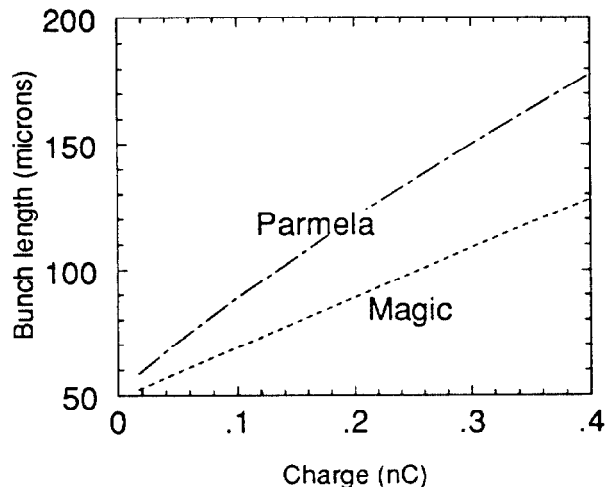


Figure 5: Bunch length at exit of RF Gun cavity.

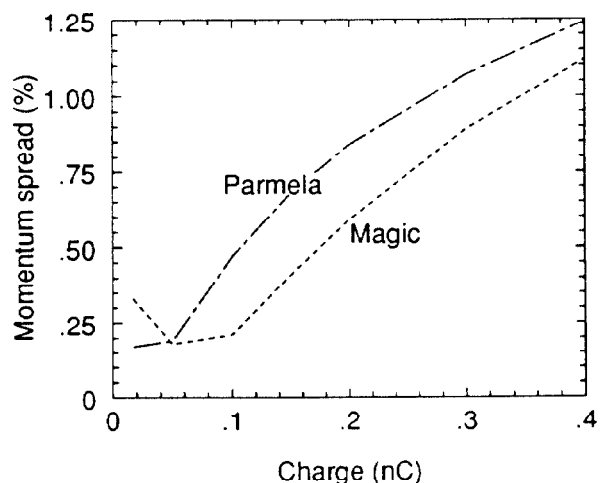


Figure 6: Momentum spread at exit of RF Gun cavity.