PARALLELIZATION OF TRACK FOR LARGE SCALE BEAM DYNAMICS SIMULATION IN LINEAR ACCELERATORS*

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Abstract

Large scale beam dynamics simulations are important to support the design and operations of an accelerator. From the beginning, the beam dynamics code TRACK was developed to make it useful in the three stages of a hadron (proton and heavy-ion) linac project, namely the design, commissioning and operation of the machine. In order to combine the unique features of TRACK with large scale and fast parallel computing we have recently developed a parallel version of the code. We have successfully benchmarked the parallel TRACK on different platforms: BG/L and Jazz at ANL, Iceberg at ARSC, Lemieux at PSC and Seaborg at NERSC. We have performed large scale end-to-end simulations of the FNAL proton driver where 10^8 particles were tracked. The actual parallel version has the potential of simulating 10^9 particles on 10 racks with 20,480 processors of BG/L at ANL, which will be available next year. After a brief description of the parallel TRACK, we will present results from highlight applications.

INTRODUCTION

The beam dynamics code TRACK [2] has been developed at ANL over the past few years. TRACK is a ray-tracing code that was originally developed to fulfil the special requirements of the Rare Isotope Accelerator (RIA) systems [2]. The code was applied for designing and commissioning of various medium energy high-intensity accelerators worldwide [4-8]. The status of the serial TRACK code has been reported elsewhere [4, 9, 10].

In this paper, we present the new parallel version of the beam dynamics code TRACK and its application for large-scale accelerator simulations. The parallel code TRACK has been used to simulate beam dynamics in the 8-GeV FNAL proton driver Linac [11], which includes a 325 MHz RFQ, a MEBT, a room temperature linac and a superconducting linac in the energy range from 10 MeV to 8 GeV [12]. The 45 mA beam at the entrance of the RFQ was represented by 100 million microparticles in a bunch. The number of particles is close to the actual number of particles per bunch and beam halo formation in both transverse and longitudinal phase spaces can be clearly observed. The choice of the number of particles is dictated not only by the space charge considerations but also by the beam behavior in combined external and space charge fields.

PARALLEL ALGORITHMS & SOLVERS

Parallel Algorithms

The code comprises two major parts: particle tracking and space charge (SC) calculation. Particles are distributed evenly over all processors for tracking while each processor has its own copy of the fields. Each processor has only part of a global mesh for the space charge calculations. The field mesh and space charge mesh are different. This scheme has the advantage of easy implementation and no communication for particle tracking is required. However, this method requires large memory in each processor and intense communication for the parallel Poisson solver.

Parallel Solvers

The Poisson solver routine used in TRACK takes beam particle distributions as input and produces the EM fields of the beam on a predefined 3D SC grid as output. The first step is to transform the particle distribution to the rest frame of the beam and perform the deposition of the electric charges carried by the beam particles (macroparticles). This is done using the so called ‘‘cloud in cell’’ method, where depending on distance, a particle deposits a fraction of its charge on the closest 8 nodes of the SC grid defining the SC cell the particle belongs to. At the end of this step the beam is represented by a space charge distribution on the SC grid. The next step consists of solving the corresponding Poisson equation for the electric potential U. We have implemented the Poisson solver in both the Cartesian and the Cylindrical coordinates with Dirichlet boundary condition in the transverse directions and periodic boundary condition in the longitudinal direction. The solution is performed using the fast Fourier transforms (FFT); sine transforms in the transverse directions and real transforms in the longitudinal direction. Once the potential U is determined on the SC grid, it is straightforward to derive the induced electric field in the rest frame of the beam. By boosting back to the laboratory frame, the EM fields could be determined on each node of the SC grid. A second order interpolation method is used to obtain the $(E; B)$ fields in the location of a given particle in the next tracking step.

1. 1D Domain decomposition in the Z direction

In this model the 3D SC grid is decomposed only in the longitudinal Z direction. Each slice in Z is assigned to a single processor. This model has the major drawback of limiting the maximum number of processors to the number of SC grid nodes along the Z direction (typically less than 256), making it useful only for a relatively small number of processors. For some applications, the simulation of very large number of macroparticles (10M to 1B) may be necessary. For this purpose, the code

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should be scalable to thousands of processors and 1D domain decomposition is not sufficient.

2. 2D Domain decomposition in X and Y directions

In this model we decompose the SC grid in the transverse plane in both X and Y directions. We choose the decomposition in X and Y directions because they are equivalent from beam dynamics point of view, which leads to a more symmetric data flow between processors. The merit of 2D domain decomposition is that it can easily be used with thousands of processors. For this we define two separate processor communication groups. One is composed of processors with the same X location called "X communicator" and the other contains processors with the same Y location named "Y communicator". This method is proved to be the most efficient one for the Poisson solver.

3. 3D Domain decomposition in X, Y and Z directions

In this model we decompose the SC grid in all three directions. Since the mesh is divided in all directions, the data transposition required before FFT is performed in the X, Y and Z directions. Three separate processor communication groups are defined. In addition to "X communicator" and "Y communicator", the "Z communicator" is defined. The advantage of 3D domain decomposition is the possibility to use larger number of processors compared to 2D domain decomposition.

4. Performance tests of the parallel models

As can be seen from figure 1 the 2D Domain decomposition has the best performance.

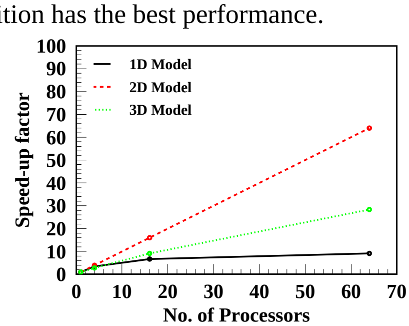

Figure 1: Scaling of 1D, 2D and 3D domain decomposition models on BG/L. The mesh is $128\times128\times256$

5. Validation of parallel Poisson solver

To validate parallel Poisson solvers, the results have been compared with known analytical solutions and the difference is within machine round-off error[1].

SIMULATION RESULTS

Comparison with the serial code

Both the serial and parallel codes were used to simulate a 325 MHz RFQ designed to bunch and accelerate a ~45 mA H^- beam from 50 keV to 2.5 MeV. Comparison for the case of 1M particles is shown in figure 2 and 3.

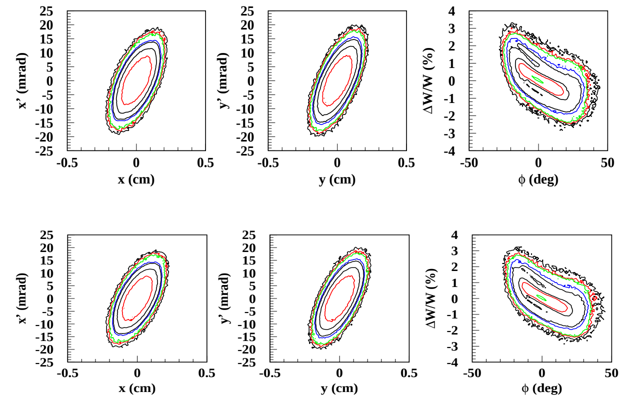

Figure 2: Comparisons of phase space contours between the serial and parallel versions of TRACK. The upper phase space plots are from the parallel code, and the lower ones are from the serial code.

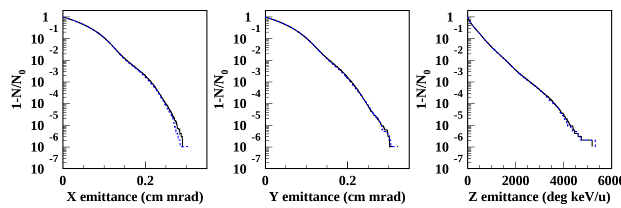

Figure 3: Emittance levels, or fractions of the beam outside a given emittance, in the three phase space planes. The solid-black curves are from the serial version and the dashed-blue are from the parallel version.

Increasing the number of particles from 100k to 1M reduces relative contribution of the SC calculations from 60% to 8% and hence improves the scaling of the global calculation, as shown in figure 4 (left). The contribution of the SC calculation is about 1% for a $32\times32\times64$ SC grid, it increases to 8% for a $64\times64\times128$ grid and to 60% for a $128\times128\times256$ grid which explains the observed reduction in scaling, as shown in figure 4 (the right plot).

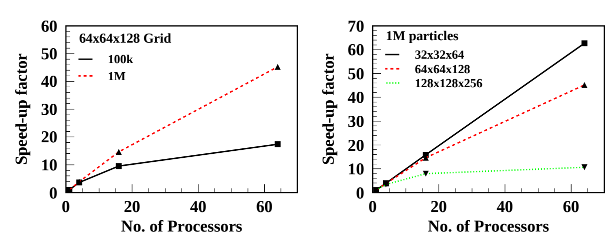

Figure 4: Left plot compares the speed-up factor for the SC grid $64\times64\times128$ and different number of particles: 100k and 1M. The right plot compares the speed-up factor for the same number of particles (1M) but different SC grids.

Large scale simulations with PTRACK

Recently we have used PTRACK for the end-to-end beam dynamics simulations of the proton driver (PD)

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being developed at FNAL [11-12]. Figure 5 compares the particle distribution for 1M, 10M and 100M macro-particles calculated following the procedure described in ref. [13]. As is seen from the figures, larger number of macroparticles results in much clear estimation of the beam halo. The comparison of beam profiles along X, Y and phase directions are shown in Fig. 6.

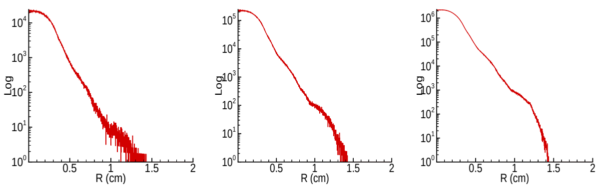

Figure 5: Comparison of the distribution for 1M (on the left), 10M (in the middle) and 100M (on the right) macroparticles.

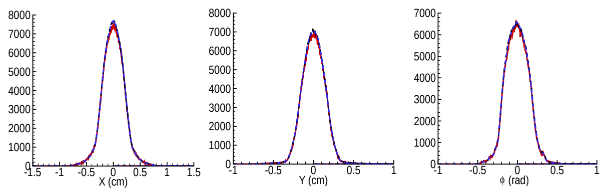

Figure 6: Comparison of beam profiles for 1M, 10M and 100M macroparticles in the X- (on the left), Y-(in the middle) and phase-directions (on the right)

Phase space plots at the end of the PD are shown in figure 7. Simulation of large number of particles reveals a significant beam halo in the $(\phi, \Delta W/W)$ phase plane which can not be seen in the low-statistics simulations.

SUMMARY

Several parallel models for solving the Poisson equation have been developed and benchmarked. The fastest Poisson solver has been incorporated into the parallel TRACK code. As an example, the parallel TRACK has been applied to study beam dynamics in the 8-GeV proton driver. Various statistical results obtained from simulation of 10^6 to 10^8 macroparticles have been analyzed. The advantage of large-scale parallel simulation of 10^8 particles has been clearly proven. The capabilities of the TRACK code have been greatly extended.

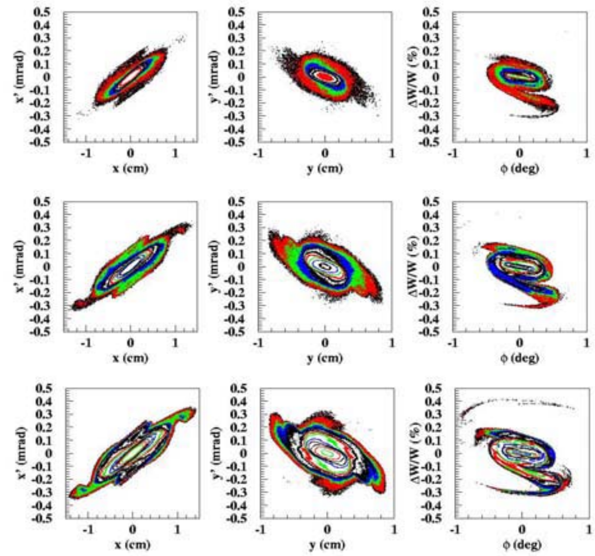

Figure 7: Phase space contours in the $(\phi, \Delta W/W)$-plane for 1M (on the top), 10M (in the middle) and 100M (on the bottom) macroparticles.

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