SIMULATIONS OF HIGH-INTENSITY BEAMS USING BG/P SUPERCOMPUTER AT ANL*

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ABSTRACT

Large-scale beam dynamics simulations are important in accelerator design and optimization. With the new BG/P supercomputer installed at ANL, tera-scale computing can be easily accessed. In order to make use of this emerging technology to increase the speed and efficiency of accelerator simulations, we have systematized and upgraded our software. In this paper, we will first introduce the new version of the parallel beam dynamic code PTRACK [1] updated to run on BG/P with more than 10^4 processors. The new PTRACK includes possibility to track ~10^8 particles through multiple accelerator seeds in the presence of machine errors. An example of SNS LINAC simulations will be presented.

INTRODUCTION

The beam dynamics code TRACK [2] has been developed at ANL over the past 10 years. TRACK is a ray-tracing code that was originally developed to fulfil the special requirements of the Facility for Rare Isotope Beam (FRIB) [2]. The code was applied for designing and commissioning of medium energy, high-intensity accelerators worldwide [5-8]. The status of the serial TRACK code has been reported elsewhere [4, 9, 10].

In this paper, we present the new developments on parallel version of TRACK code, PTRACK and its new applications for large-scale accelerator simulations. The parallel code PTRACK has recently been updated to have more systematic structure, and 3D domain decomposition parallel Poisson solver has been added to it. This makes it possible to simulate real number of beam particles in the 325 MHz Radio Frequency Quadrupole (RFQ). It has also been used to simulate 100M particles through Fermi Lab. Proton driver linac in the energy range from 2.5 MeV to 8 GeV [11]. The number of particles is equal to the actual number of particles per bunch.

NUMERICAL METHODS

Particle-In-Cell (PIC) method has been adopted in TRACK code. 4th order Runge-Kutta scheme has been adopted for time integration. The external EM fields are provided by commercial software, like MWS, ANSYS, etc. The space charge effect is included by solving Poisson's equation. Several Poisson solvers have been developed in both Cartesian and Cylinder coordinate systems, and domain decomposition has been used for parallelization. Detail information can be found in [1, 6, 10].

* This work was supported by the U.S. Department of Energy, Office of Nuclear Physics, under Contract No. DE-AC02-06CH11357.
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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 Poisson 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 (macro particles). 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, 2D and 3D Domain decompositions in Cartesian coordinate system

As shown in Fig. 1, three parallel models have been developed in Cartesian coordinate system. The merit of 2D and 3D domain decomposition is that they can easily be used on tens of thousands of processors. Different communication groups need to be generated to transpose

operation. The advantage of 3D domain decomposition is the possibility to use larger number of processors compared to 2D domain decomposition.

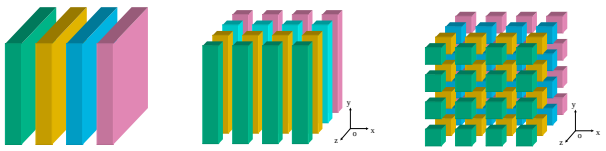

Fig. 1: 1D, 2D and 3D domain decompositions for parallel Poisson solver in Cartesian coordinate system

2. 2D Domain decompositions in Cylinder coordinate system

Figure 2 (left) shows the 2D domain decomposition model for parallel Poisson solver in Cylinder coordinate system.

3. Parallel Poisson solver Benchmarks

As can be seen from Fig. 2 (right) the 2D Domain decomposition has the best performance. This may be due to the small grid used for SC calculation.

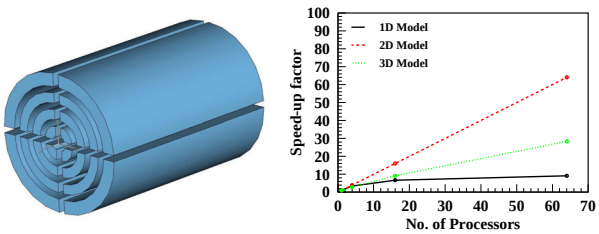

Fig. 2: 2D domain decomposition model in Cylinder coordinate system (left) and Scaling of 1D, 2D and 3D domain decomposition models on BG/L. The mesh is 128×128×256 (right)

LARGE SCALE COMPUTING

Advantages

- Provide more advanced support for accelerator science, reduce cost for accelerator design, commission and operation.
- Can overcome shortcoming of PIC method by simulating real number of particles
- More accurate and detailed simulations, important to investigate more complicated phenomena, such as halo, beam losses, etc.
- Speed up simulations and shorten simulation time
- Study more misalignment errors by simulating larger number of particles and seeds to improve the LINAC designs
- Investigate more challenging problems which can lead to new scientific discovery!

Challenges

As the processor number increases, there are many challenges associated with large scale computing. I/O is one of these. Suppose we perform I/O on each processor, using 32k files into one directory will cause problem. Subdirectories need to be created to overcome this. Another challenge is load balancing on BG/P system, as each processor only has 512MB memory. Well balanced code need to be developed to run on BG/P system. The most challenging problem is post-processing, as 160GB data will be generated using 32k processors, transferring and post-processing both take large mount of time. Therefore, we have developed parallel post-processing code to analyze these large mount of data. Further development are definitely needed in the future. 2D and 3D parallel Poisson solvers show their advantages with 32k processors, as the smallest grid can be used for 2D model is 128×256×128, while 3D model is 32×32×32. The large mount of data usually reaches hundreds of GB, all these need advanced hardware and software systems.

BENCHMARK AND SIMULATION RESULTS

Large Scale Benchmarks

Both the weak and strong scaling results has been shown in Fig. 3. For weak scaling, we increase the particle numbers from 55M to 880M on 256 to 4096 processors. This keeps the particle number constant on each processor. The simulation time is also nearly constant as can be seen in the Fig. 3 (left). For the strong scaling in Fig. 3 (right), we simulated 110M particles on 512 to 4096 processors, and good scaling has been demonstrated. Table 1 shows I/O and total time for simulating different number of particles using different number of processors. The I/O time to simulate 865M particles on 32k processors is only about two minutes, and total time for 269 cell RFQ is about 6 hours.

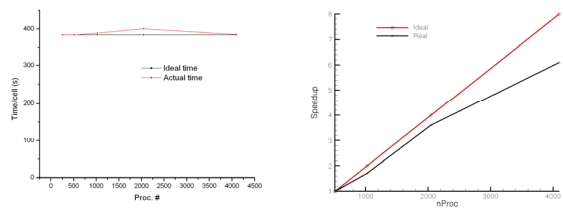

Fig. 3: Weak (left) and strong (right) scaling for PTRACK code.

Table 1: Comparisons of simulations with different numbers of particles

Particle#	1M	10M	100M	865M
CPU#	1024= 16*16*4	4096= 16*16*16	4096= 16*16*16	32768= 32*32*32
Particle/CPU	1k	2.56k	25.6k	26.4k
SC Grid	(32,32,32)	(32,32,32)	(32,32,32)	(32,32,32)
I/O time(s)	14	110	36	135
Tot Time(h)	0.63	1.06	6.3	5.8

Simulation Results

Increasing the number of particles from 100k to 1M reduces ratio of SC to particle tracking time from 10% to 3.7% and hence improves the scaling of the global calculation, as shown in Fig. 4 (left). The ratio of SC to particle tracking time is about 3.7% for a 32×32×64 SC grid, it increases to 8.6% for a 64×64×128 grid and to

60% for a 128×128×256 grid which explains the observed effects in scaling, as shown in Fig. 4 (right).

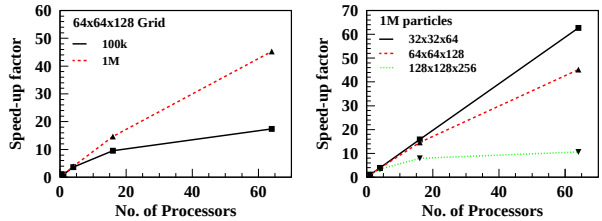

Fig. 4: Left plot compares the speed-up factor for the SC grid $64\times64\times128$ and different number of particles: 100k and 1M. The right plot compares the speed-up factor for the same number of particles (1M) but different SC grids.

Large scale simulations with PTRACK

As preliminary effort, real number of particles have been simulated through 30 cells in Radio Frequency Quadrupole (RFQ) using 32,768 processors. Figure 5 compares emittance levels with 1M particles. Longer tails in the plots give more information on particles distribution in phase spaces. Figure 6 shows the phase contours in (x, x'), (y, y') and $(\phi, \Delta W / W)$ planes.

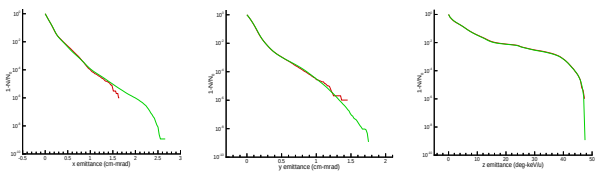

Fig. 5: Emittance levels, or fractions of the beam outside a given emittance, in the three phase space planes. The red curves are 1M particles and the green curves are 865M particles.

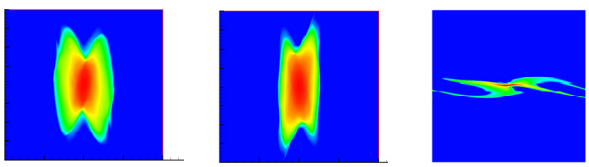

Fig. 6: Phase space contours in the (x, x'), (y, y') and $(\phi, \Delta W / W)$-phase planes for 865M macroparticles.

We also used PTRACK for the end-to-end beam dynamics simulations of the proton driver (PD) being developed at FNAL [11]. As shown in Fig. 7 (left), detailed statistics can be analysed for full PD driver. The right plot in Fig. 7 shows the number of lost particles at different locations, this demonstrates the advantage of large scale computing. It is hard to find lost particles by simulating small number of particles. This simulation only takes about 6.5 hours using 4k processors.

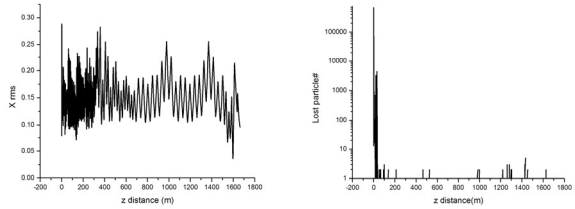

Fig. 7: 100M particles Xrms statistics through full Fermi Lab. PD LINAC (left), Lost particle numbers (right).

With PTRACK being successfully ported on BG/P, large scale computing could be conducted on other LINAC, such as SNS, ATLAS, FRIB, etc. Large scale optimizations also become possible by the fast speed of PTRACK.

SUMMARY

PTRACK code has been updated and successfully run on BG/P system. In order to include space charge effect, several Poisson solvers have been developed in both Cartesian and Cylinder coordinate systems. They have been parallelized by domain decomposition method. Good scaling has been demonstrated using large number of processors. The advantages and challenges of using tens of thousands of processors for large scale computing have been discussed. The capability of simulating real number of particles through LINAC has been presented. Simulation of 100M particles through 8-GeV Fermi Lab. proton driver has been conducted. The capabilities of the PTRACK code have been greatly extended. With upcoming full instalment of BG/P system at ANL, PTRACK can greatly improve the beam dynamic simulations of LINAC system.

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