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UPGRADES ON A SCALABLE SOFTWARE PACKAGE FOR LARGE SCALE BEAM DYNAMIC SIMULATIONS

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Abstract

Scalable software package for beam dynamics simulation are playing more and more important role in precise design and optimization of the linear accelerator. In this paper, recent upgrades (version 2.0) on LOCUS3D, which is a parallel software developed for beam dynamics simulation, are introduced. The numerical methods are kept as before, but whole structure of the software has been rebuilt. These upgrades include optimized software structure, more reasonable arrangements of components, and capability of simulating several different kinds of particles with different charge states and masses. It also provides suitable structures for extension to use modern heterogeneous supercomputers. Standard accelerator devices have been tested again for this new version. The new software can run on several different platforms, such as INSPUR cluster, TIANHE-2, and BG/P at ANL. At last, some simulation results for DTL with large number of particles will be shown.

INTRODUCTION

Many beam dynamics codes [1-5] have been developed for beam dynamics simulations, but few of them were designed and developed specifically for efficiently use of the newly emerged software and hardware technologies for large supercomputers. LOCUS3D [6] was developed for meeting this purpose in 2013. It solves the Poisson's equation for the space charge effect, and the time integration algorithm uses sub-steps for effects of electric and magnetic fields separately. After several years of successful simulations, several places need improvements to meet more broad requirements.

In this paper, we explain several upgrades on the LOCUS3D. These upgrades include new data structure, software structure, and future extension for heterogeneous supercomputers. The new data structure setup new relations between different elementary classes, such as PtcSet, Bunch, Device and Solver etc. The new relation is based on natural relation between these concepts, which make them easier to be used for building applications in BDS. The new software structure separates functions based on different classes by different levels. High-level functions are built on low-level functions, and are made from them. Furthermore, new software structure provides extension, which can easy use the heterogeneous supercomputers in the future. These upgrades require new particle initialization module, time integration module, Poisson solver module, parallel model and parallel I/O module. The new version has been tested to simulate beam dynamics in the basic accelerator devices, such as multi-pole lenses, solenoid, and Drift Tube Linac (DTL). The parallel Poisson solver has been successfully redeveloped and benchmarked on the new Solver class. Besides the FFT Poisson solver, other numerical methods can easily build alternative solver under new software structure. This upgrade makes LOCUS3D more suitable to meet various demands exist in design and modelling of linear accelerators. Accelerator physicists and engineers can easily have features that satisfy their requirements. The paper will introduce the new data and software structure first, and then give benchmark and simulation results.

NUMERICAL METHOD

The numerical methods are similar, and can be divided into two parts: particle tracking and electromagnetic (EM) field computation, including external fields and space charge (SC) fields. Particle tracking is designed to have different time integration schemes for choices [7], which can be realised easily based on the new software structure. A parallel Poisson solver using Fast Fourier Transform (FFT) [8] has been developed for SC field computation. Currently LOCUS3D uses sub-steps to separates the effects of electric and magnetic fields, which is similar to the algorithm of BEAMPATH code. But it has many differences from B6EAMPATH, such as units of quantities, Poisson solver, parallel model, etc. Detail information can be found in our previous paper, which will be omitted in the following sections.

UPGRADE STRUCTURES

LOCUS3D was designed from beginning to be parallel software for complete beam dynamics simulations. It is based on MPI library, and object-oriented C++ language. It targets on modern supercomputers, such as TIANHE, BG/P, etc. After several years of successful running, we are upgrading it for many places in order to make its structure more reasonable in nature, easier for extension for simulating complex physics and for using modern supercomputers.

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Data Structure

The most elementary class of LOCUS3D is the BUNCH. In order to handle bunch consisting of particles, which may have different charge states and masses, the upgrade version introduces the class PTCSET, which represent single bunch with specific charge state and mass. Then the class BUNCH can be defined with several variables of class PTCSET. As shown in Fig. 1, the class PTCSET consists of class PHASE for single particle. The class PHASE is defined with 6 variables for the position and momentum of each particle. Their memories have been allocated in class BUNCH, which make them easy to access in large scale computing. Specific features of C++ language have been utilized to make them scalable and extensible.

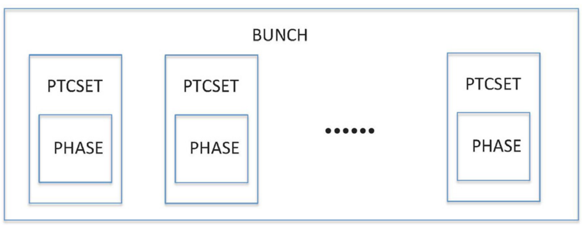

Figure 1: Relation for class BUNCH and others.

In Fig. 2, the relation of primary classes has been shown. As can be seen, each BUNCH class has a function, INIT, which initialise the bunch distribution. On each CPU, class DEVICE has all information of various devices in the accelerator, and class PARAM has all parameters read from input file. These two classes have same copies on all processors. By helping of MPI functions, two important classes are created. They are POISSON SOLVER and STATISTICS. The new upgrade has redeveloped all these two classes based on the modification of class BUNCH for counting the multiple charge states and masses.

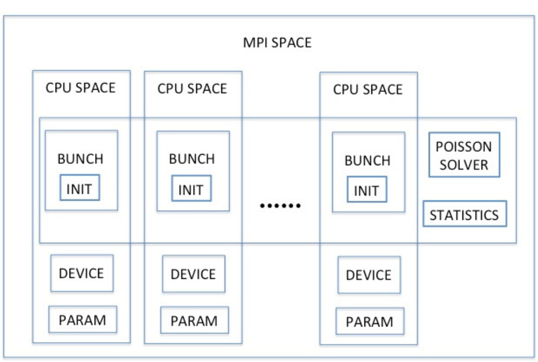

Figure 2: Relation of primary classes in LOCUS3D-2.0.

Software Structure

During past several years, it is shown that the software structure of LOCUS3D needs some improvements to meet more broad requirements in the simulations. This makes upgrade to have completely new software structure than original version. Three levels have been formed to handle different operations. The first level handles the fundamental I/O for particles, variables and parameters. The second level is the primary part for the new version, which has several parts to handle different components. This makes the software structure clear to understand and extend. The third level is the highest level, which handles different numerical methods for the BDS.

Parallel space charge field solver is used to solve the static electric field $\boldsymbol{E}$ in equations $\nabla^2\phi=-\rho/\varepsilon_0$ and $\nabla\phi=-\boldsymbol{E}$, and the related class diagram of C++ code is shown in Fig. 3. Class *Fourier*, *PotentialFourierSolver*, and *FieldSolver*calculate the Fourier transform of ρ, the Fourier transform of ϕ, and $\boldsymbol{E}$ respectively. *MapReducer*is responsible for the map and reduce of charge density data and electric field data of the particle-in-cell grid.

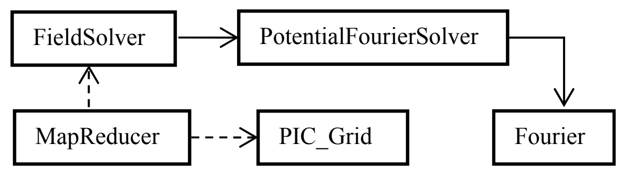

Figure 3: Class diagram for solving space charge field.

Under these new data and software structures, LOCUS3D can easily make use of modern hardware of supercomputers. The new upgrade is easy to add flexible extensions to handle more complex physics and computer techniques in the future.

VALIDATION AND SIMULATION

Validation

Standard devices, such as multi-pole lenses, bending magnets, solenoids and DTLs, have been simulated with the upgraded version, and identical results as before have been obtained. This validates the correctness of the upgraded version.

Simulations

Next, a combination of DTL and solenoid focusing has been simulated with the new upgraded version, and same results have been obtained as before. The DTL consists of 157 gaps with frequency 85.7 MHz. 10^5 particles have been used in the simulations below.

Growth of the average energy along the DTL is presented in Fig. 4. The result matches those of BEAMPATH very well. Emittance variation along the DTL is presented in Fig. 5, which shows that they are nearly constant at latter part of DTL. The envelope variation of the horizontal vane and vertical plane along the DTL are presented in Fig. 6, which are similar to the emittance growth.

Large scale particle tracking with 1 billion macro particles have been carried out by the upgraded version.

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Table 1 shows the scalability on TIANHE-1 and Table 2 shows the scalability on TIANHE-2. From them, upgraded version has good scalability when using large number of processors.

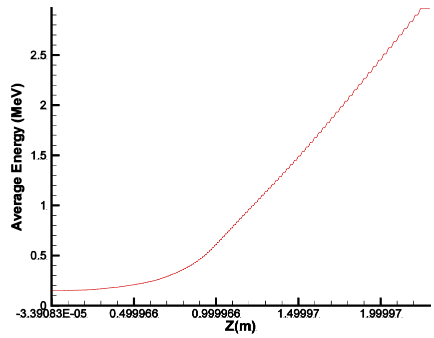

Figure 4: Growth of the average energy along the DTL.

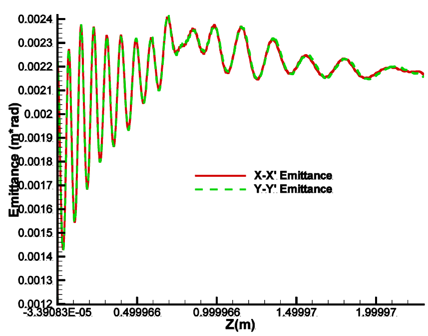

Figure 5: Emittance variation along the DTL.

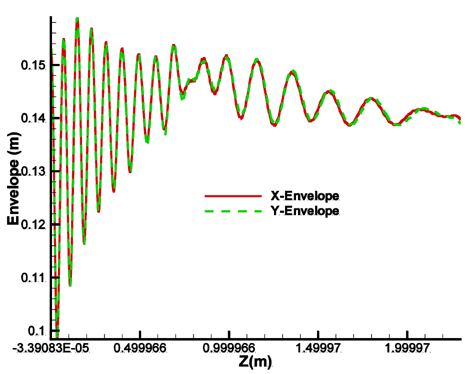

Figure 6: Envelop variation of the horizontal and vertical along the DTL.

Table 1: Benchmarks on TIANHE-1

CPUs	1M/CPU, time (s)/PE	16M total particles, time (s)/PE
4	15.9/100%	253.9/100%
16	16.3/97.5%	63.8/99.5%
64	16.0/99.4%	16.3/97.4%

Table 2: Benchmarks on TIANHE-2

processor no.	particle no. (M)	time per step (s)
64	16	5.92
256	64	5.97
1024	256	5.96
4096	1024	5.93

SUMMARY

This paper presents recent upgrades on parallel beam dynamics software, LOCUS3D, which was developed before. The purpose is to meet more broad demands from different groups of users. The upgrades include software structure optimization, more reasonable arrangements of components, and capability of simulating several different kinds of particles with different charge states and masses. These upgrades make LOCUS3D more scalable and extensible on modern supercomputers. Benchmarks are shown on TIANHE-2. A DTL with solenoid accelerator has been simulated, and accurate and useful information have been obtained. Optimization and extensions will be made continuously to make LOCUD3D more powerful in the future.

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