On the Way to Future’s High Energy Particle Physics Transport Code

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Abstract—High Energy Physics (HEP) needs a huge amount of computing resources. In addition data acquisition, transfer, and analysis require a well developed infrastructure too. In order to prove new physics disciplines it is required to higher the luminosity of the accelerator facilities, which produce more-and-more data in the experimental detectors.

Both testing new theories and detector R&D are based on complex simulations. Today have already reach that level, the Monte Carlo detector simulation takes much more time than real data collection. This is why speed up of the calculations and simulations became important in the HEP community.

The Geant Vector Prototype (GeantV) project aims to optimize the most-used particle transport code applying parallel computing and to exploit the capabilities of the modern CPU and GPU architectures as well. With the maximized concurrency at multiple levels the GeantV is intended to be the successor of the Geant4 particle transport code that has been used since two decades successfully. Here we present our latest result on the GeantV test performances, comparing CPU/GPU based vectorized GeantV geometrical code to the Geant4 version.

Keywords—High Energy Physics, High Performance Computing, particle tracking, numerical simulation, computer simulation, vectorized Geant, GeantV

I. INTRODUCTION

High Energy Physics (HEP) requires a significant amount of computational resources at several layers of the data taking processes. Detector upgrades of the experiments generate further needs for the computational capacity of hardware, software, and middleware levels. Since the increase of the CPU-clock frequency saturated a few years ago, developers turned to push more effort for the software-development side in order to exploit all the capabilities exist in the parallel architectures and many-core computing.

Early performance analysis of the detector and theory simulations have been already explored the bottleneck of the numerical calculations, which found to be the particle transport – the most time-consuming part of the simulations. Due to this reason the investigation of the possibility to rebuild the most widely used particle transport framework, Geant4 (GEometry ANd Tracking), in a vectorized/parallelized way was started [1-16].

Recent version is the Geant4 simulation framework, which is used by most of the experimental collaborations of the Large Hadron Collider (LHC, CERN) and many others all around the world. Its main purpose is to simulate the passage of particles through matter using Monte Carlo methods. The development of the original simulation package started in 1994, and since 2012 studies for the possible successor, the Geant Vector Prototype (GeantV) project has started [1, 2, 17]. The Geant development was always a worldwide collaboration and it has many application areas outside of particle and nuclear physics, such as: space science, nuclear reactor development, or medical/radiological fields.

The basic idea of a parallel version of these simulations lays on the vectorized geometry calculations. The already vectorized GeantV code executes single instructions on multiple data (SIMD) in parallel. A relevant speedup has already achieved on CPU architectures which supports vector instructions.

Nowadays, it is a popular trend to transform numerical codes to able to run on the fast, General-Purpose computing on Graphics Processing Units (GPGPU) [18]. This fashion fits nicely to the strategy of GeantV development, since geometrical computations with GPUs are pretty effective, especially in cases where the size of the input to be processed is big compared to the CPUs. In the case of HEP geometric calculations for all particles are independent, thus it is reasonable to prepare the particle transport code for such cases and implement the support for GPUs or other many-core architectures.

The VecGeom library (Vectorized Geometry) is the geometry package which was started to develop in the context of the Geant Vector Prototype project in 2013 [2, 3]. By the time it will be finished, this became a standalone library that provides a GPU support via the Computer Unified Device Architecture (CUDA) compiler as well. This CUDA backend already exists in VecGeom, which supports only NVIDIA devices at the moment. On the other hand we investigated how could we increase the portability and the performance on multiple architectures, with the usage of the Open Computing Language (OpenCL) framework [19].

In this paper first we give a general overview of the Geant framework, then we introduce the generalization of the particle transport simulation. Finally we show the speedest results of VecGeom on CPU and GPU architectures and present the comparison between them.

*See the Appendix for the list of the collaboration members.
II. PROJECT GOALS

We introduce the general aims of the GeantV project focusing on the parallelization and vectorization.

A. New generation of particle transport simulations

The famous Moore law stated in the ’60s says that the number of transistors integrated on one single chip grows exponentially with time [20]. The scaling law presented on Fig. 1 is still valid in hardware sense. Although relevant speedup has not been achieved recently, because the clock frequency of the CPUs has reached the currently maximal value of 3-4 GHz since the middle of the last decade. Due to the increasing number of CPU cores per chip and other advanced architecture technologies the computing performance still able to be increased, but the exploitation of this increasing performance needs new, so far not widespread programming techniques. Since the popularity of video games increased recently, the graphical hardwares (GPUs) were greatly improved. Today these hardwares become suitable and used even for scientific calculations [3, 17, 18, 21–23].

The power of the computing performance may not appear by increasing the clock frequency, but in the utilization of parallelization and vectorization. The parallel computing with CPUs has long history. The first SIMD instruction set appeared at late ’90s, however in the last few years the new generations of CPUs have more-and-more advanced SIMD support (SSE4, AVX-512) and therefore they are becoming more effective with a vectorized software. The outline of the operating principle of the SIMD instructions is seen on Figure 2.

The main goal of the Geant Vector Prototype Project (GeantV) is to exploit the benefits of the modern CPU, GPU and many-core architectures at the same time. The project started in 2012 with preliminary performance analysis which showed that in a typical detector simulation the geometry calculations itself using major of the computational resources, 40 − 50% in time [11]. On the other hand, geometry calculations are independent of each other, which gives an hand-on opportunity for parallelization. The layout is seen on Figure 3 where scheduler manages geometrical algorithms and physical processes [3, 5, 17].

![Fig. 1. The famous Moore law says that the number of transistors integrated on one single chip grows exponentially with time [20]. However, it is still valid in hardware sense, but significant computational power has not been achieved so far due to the CPU-clock speed saturation on 3-4 GHz [24].](image1)

![Fig. 2. Left panel: A scalar code performs one operation per CPU-tick, while a vectorized, SIMD-instruction based operation is capable to make the same operation on a data vector at the same time (right panel).](image2)

![Fig. 3. The structure of the GeantV prototype: scheduler manages geometrical algorithms and physical processes [5, 17].](image3)

Development of the code aimed to get maximal performance beside maintainability and hardware independence. On the top of this, the predecessor, Geant4 is developed and used since two decades and the successor has to be suitable for long term as well. Thus the software has to be compatible not just with the older hardwares but with future ones too. Following Fig. 3 the development of GeantV has three different levels:

1) Scheduler: While in Geant4 the particle transportation happened serially, GeantV will manage multiple particles at the same time. Because the transportation is a local process and most of the simulation steps occur in a small part relative to the whole detector geometry, the main idea was to collect the particles which are in the same type of volume into vectors (baskets) and perform computations parallel using SIMD instructions. In this way both the necessary memory containing the different parts of the detector, and the necessary computational time can be strongly reduced. The scheduler manages the baskets of particles as an interface between the physics and geometry.

2) Physics: At present the physics of GeantV is tabulated, which means that instead of theoretical calculations the physical processes are pre-calculated and ordered in multidimensional tables. Because in this way all the possible final states are given in advance, the necessary computational time can be strongly reduced. The scheduler manages the baskets of particles as an interface between the physics and geometry.
well. For higher precision one should pre-calculate and load more final states, requiring more memory. The physics of the final version of GeantV is still in the design phase.

3) Geometry: In a particle transport simulation a very significant part of the runtime (40-50%) is devoted to the geometrical calculations. Therefore it is important to take advantage of the most computational capacities of the hardware in the implementation of the geometry code. The main purpose of the VecGeom (Vectorized Geometry) package is to use more efficiently the different hardware architectures via vectorization.

III. HIGH PERFORMANCE COMPUTING IN HEP

In parallel to the development of detector- and data-acquisition technologies computing architectures went through a major a evolution during the last years too. In order to keep the scientific advancement, the necessary infrastructure needed to be improved following the construction of the huge particle accelerators and giant detector systems. This trend is still ongoing: the hardware manufacturers release the newer and better hardwares regularly – sometimes motivated by the needs of the HEP community.

As we have mentioned earlier, in Geant4 in high-energy physics simulations the detector-particle interaction uses the main computational-resource part. Moreover any detector-simulation and -design require particle transport simulations especially, one need to calculate the detector efficiency or perform predictions by theoretical calculations. We note, besides HEP applications several other disciplines are also served such as medical applications or space sciences, where there is a need to simulate the transport of particles through matter.

In a transport simulation the most significant quantity regarding the computational time is the number of steps. While the particle passing the matter, it will interact with its environment many times, and the distance between two interactions called step length. For a given process, this length is determined by the mean free path, \( \lambda_i \), which is calculated by the following formula:

\[
\lambda_i = \frac{1}{n \sigma_i} ,
\]

where \( \sigma \) is the total cross section of the given process and \( n \) is the density of the medium. The total cross section is the sum of the cross sections for all processes:

\[
\sigma_{total} = \sum_i \sigma_i .
\]

If the size of mean free path is large (e.g. in vacuum), the step length can be large as well, so one may needs only a few steps until one can eliminate the particle (when it leaves the range of interest). On the other hand if the mean free path is small, it means that interactions take place even in short distance. In this case one needs more steps with smaller \( \lambda_i \), which require more computational time to simulate the same distance at the same precision. The inverse of the mean free path equals to the inverse sum of the mean free path of all the possible interactions:

\[
\frac{1}{\lambda_{total}} = \sum_i \frac{1}{\lambda_i} .
\]

The two main parts of a Geant4 particle transport simulation are physics and geometry.

A. Physics

For a given particle type at fixed energy it may happen different kinds of interactions. One can distinguish the following three types:

- **At rest**: It occurs when the kinetic energy of the particle is zero. The selection criteria in the case of the at rest processes is the lifetime of the particle (e.g. radioactive decay).
- **Along step**: Processes which happen during the transportation (e.g. ionization).
- **Post step**: The processes which take place after one step, after the transportation has been fully completed. This depends on the interaction length (e.g. elastic scattering).

The process which is being implemented in the actual step is selected by the lowest mean free path. In the first step the code calculates all the possible mean free paths via Monte Carlo method for all the possible interactions at a given energy. In the next step the shortest mean free path will be implemented. If the lowest mean free path is larger than the distance from the geometric border (which is the boundary layer of two volume with different materials), then the particle is being transported to the border. In the next step the mean free paths will be calculated with the material of the new volume.

These two methods (the calculation of the physical interaction length (GetPhysicalInteractionLength) and the execution of the step (DoIt)) are implemented in every steps. During a simulation the tracking of a particle is ended when its energy becomes lower than a given threshold or it decays, or it leaves the investigated geometry. The execution of a step (transportation and the implementation of the processes) is calculated with Monte Carlo methods as well.

B. Detector geometry

Complex detector systems are built with basic three dimensional geometric units like rectangular solids and tubes. The fundamental geometric calculations, like coordinate transformations and distance calculations are implemented in the source code of these elementary bodies. Using boolean operations one can construct complex, composite elements as well. Finally with hierarchical connections one can build the whole detector geometry as an ordered system of the basic building blocks. The geometric calculations, like e.g. distance calculations, do not depend on the particle type. This one of the most computational intensive tasks, since it has to be carried out in every step. Thus it is crucial to implement them in an efficient and fast way.
The time is determined by the number of steps. In Geant4 the simulation is serial, which means that it tracks all the particles individually, one after the other. This results that the running time of the simulation will be proportional to the number of the particles. Since the simulation of the large detector systems need a huge amount of resources, the next generation of particle accelerators and detectors require to develop the new generation of particle transport simulations. For example: the simulation of one single particle in the ALICE detector system needs a few ∼ms, while in the LHC there are particle collisions and particles to be detected in every ∼ns.

C. VecGeom

The VecGeom library is the vectorized geometry package of the GeantV which is devoted to speed up the code of the elementary three dimensional solids and the basic calculations: rotations, translations, logical operations, and distance calculations \[2, 3\]. During a simulation there are three questions to be answered for all the particles:

- Is the particle inside or outside the solid?
- What is the minimal distance between the particle and the border of the solid?
- What is the maximal step length for a particle with a given velocity and direction?

The purpose of VecGeom is to answer these questions as fast as possible with parallelized calculations. The main idea is to collect all the particles which are located in the same type of volume and perform the calculations for all of them simultaneously with SIMD operations. In addition, the same operations have to be executed with different architectures, while minimizing code duplication. Using of template classes the VecGeom library is able to run the same code on either CPUs or GPUs even with or without vector instructions.

For vectorization on CPU architecture one may have multiple choices. The VecGeom uses the Vc SIMD library to perform explicit vectorization \[25\]. Thereby the code will be always vectorized regardless of the compiler. In order to use the same code on GPU architectures the VecGeom uses CUDA platform which works very nicely with the CPU vectorized C++ code too. A further option can be the OpenCL (and SYCL) version, which is under construction \[19\].

In order to present the power of the VecGeom library, we performed a speed test of two bodies, a Box and a Tube, presented on Figure 4. During the test the speed of the DistanceToOut method were measured, which gives the distance of randomly placed particles with random speed escaping from the bodies. Fig. 4 shows the relative speedup to the Geant4 calculations as a function of the number of particles and the vertical axis shows the speed of the calculations. In order to reduce the statistical fluctuations the calculations at a fixed particle number was repeated 5000 times.

The tendency of the tests is clearly visible: in case of CPU calculations a relevant speedup were measured even with low particle number, while in case of GPU to higher the particle number increase the speed of the calculations.

Fig. 4. Speedtest of the VecGeom Box and Tube bodies - the used hardwares are an Intel Core i7-920 CPU (SSE4.2 instruction set) and a NVIDIA Tesla C2050 computing processor \[26\].

IV. Conclusion

Since future HEP facilities require more-and-more speedup both by hardware and software way, the development of the next generation of GEometry ANd Tracking (Geant) code for many-core architectures was started. The aim is to build the vectorized GeantV code able to manage several times speedup calculations either on CPU and on GPU architectures. Here we presented the first promising results with the VecGeom library for simple body (Box and Tube) cases which were done in collaboration with the CERN PH-SFT group during a CERN Summer internship in 2014.

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Appendix

The GeantV Collaboration

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