

GEANT-4 GPU Port:

Software Requirements Specification

Volere Template, Edition 16

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1 Revision History

Table 1: Revision History

Description of Changes	Author	Date
Initial draft of document	Stuart, Matthew, Rob, Victor	2015-10-05

2 Project Drivers

2.1 Purpose of Project

2.1.a Project Background

Currently running GEANT4 simulations that require many particle takes a long time to compute when run on the CPU. By running the simulation on the GPU the user should be able to see a significant speed up in computation times

2.1.b Goal of the project

The goal of this project is to port the GEANT4 code to be able to run on the GPU.

2.2 Stakeholders

The stakeholders that are currently involved with the project include: the project group, the supervisors of the project, as well as the McMaster Engineering Physics Department.

2.2.a The Client

The client(s) for the project is the Dr. Buijss and his Grad Student Westly, representing the McMaster Engineering Physics Department. The clients proposed the project because they have invested interest in running GEANT-4 simulations more efficiently. They will be using the parallelized code to run and study nuclear simulations, and need the code to run much more quickly to obtain useful data.

2.2.b The Customer

The customer in this case also includes the client; and as such they will be the part of the end-user group that we will cater to. The customer is also other members of the Engineering Physics department who wish to run simulations using GEANT-4 as they also have use for the end product. The users will want to run simulations with many particles and particle collisions, the optimization of the code will allow for them to do this in a timely fashion.

2.2.c Other Stakeholders

The project group members hold stake in the successful completion of the project. If the project is done well, and the documentation is error free and concise, they are bound for high grades in their course.

Collaborators and users of the GEANT-4 project could be potential stakeholders, but only if after the project is completed, they accept our contributions to GEANT-4.

2.2.d The Hands-On Users of the Product

Undergraduate and graduate students as well as professors in the McMaster Engineering Physics Department would be hands on users of the product.

2.2.e Personas

Consider Matt Douglas, a graduate student in the Engineering Physics Department. Matt needs to see how a nuclear reactor would start given some specific starting conditions, and a close to realistic number of particles. Matt isn't particularly fluent in C, but he can manage to change some starting variables. Matt inputs his desired number of particles and specific starting conditions into a GEANT-4 simulation. The simulation runs for several hours before Matt realizes that it might be too much for his software and hardware setup. He finds a version of GEANT-4 written for NVIDIA GPU's that claims to speed up a simulation on average 400x. He installs this version of GEANT-4 and attempts his simulation again. This time it takes only a half hour for his simulation to yield results.

The project will help not only graduate students like Matt, but undergraduates as well. It is as useful as a learning tool as well as for research projects.

2.2.f Priorities Assigned to Users

Priority will be given to Wesley, the grad student that proposed the project to Dr. Buijss. He will be the first and main user of GEANT-4 after it is running in parallel.

3 Project Constraints

3.1 Mandated Constraints

There are global constraints put in place by the existing software, the stakeholders, and the structure of 4ZP6. The project must be built upon the existing GEANT4 code. The final product must be able to run any code/simulation that ran on the existing software. The software must run in parallel on an NVIDIA GPU. Additionally, the final product needs to be completed by the end of April, 2016. If these global constraints are not met the final product is not acceptable.

3.2 Naming Conventions & Terminology

Throughout the document, “the project”, “the product”, and/or “the software” all refer to the modified GEANT-4 code that will include the capability to be run on a GPU. The “existing software” refers to the current GEANT-4 simulation toolkit.

3.3 Relevant Facts and Assumptions

3.3.a Facts

- GEANT4 is programmed in C++
- GEANT4 runs simulations on CPUs
- Simulations run calculations on each particle independently

Table 2: Glossary

Term	Description
GEANT-4	open-source software toolkit used by stakeholders to simulate the passage of particles through matter
GPU	graphics processing unit, well-suited to parallel computing tasks
GPGPU	concept of running “general-purpose” computations on the GPU
CUDA	parallel computing architecture for general purpose programming on GPU, developed by NVIDIA

- Calculations on each particle are relatively simple probabilities

3.3.b Assumptions

- The user will have a strong understanding of particle physics
- The user will know how to use GEANT4

4 Functional Requirements

4.1 The Scope of the Work

4.2 Business Data Model & Data Dictionary

Because of the nature of our product, all data that is relevant for operation is identical to the data germane to GEANT4. This includes the world geometry of the simulation and properties of all particles (momentum, location, etc). Because our software is concerned only with data specific to GEANT4, this section is not applicable.

4.3 The Scope of the Product

The following table outlines the use cases for the product. Click the PUC # to go to its description.

Descriptions of each PUC, referenced by PUC # are as follows.

Table 3: Product Use Cases Summary

PUC #	PUC Name	Actor(s)	Input/Output
1	Simulating Particles	Researcher	Simulation parameters (in), Distribution of particle's locations (out)

1. The software will be used by researchers wishing to simulate large numbers of particles interactions with materials. The researcher sets simulation parameters, including the number of particles, their lifetime, and the material properties before running the simulation. On completion, the program gives back a map of where each particle travelled, so researchers can study where the particles are most probably to end up.

4.4 Functional Requirements

Req. #: 1	Req. Type: 4.4	Use Case #: 1
Description: Particle computations run on the GPU		
Rationale: Design requirement, will allow particle simulations to run faster (requirement 5)		
Fit Criterion: Running the product with GPU computation enabled will result in all computations on particles being offloaded from the CPU (existing product) to the GPU (new product)		
Priority: Very High		History: Created September 29, 2015

Req. #: 2	Req. Type: 4.4	Use Case #: 1
Description: Changing existing projects to run with new GPU functions should be easy		
Rationale: Design requirement, the user is able to easily choose to run old or new projects on the GPU.		
Fit Criterion: User should be able to quickly enable GPU computations by referencing the documentation. If their hardware is compatible, their project should run with no errors.		
Priority: High	History: Created September 29, 2015	

Req. #: 3	Req. Type: 4.4	Use Case #: 1
Description: Existing projects should not be affected by the new code. By default, they will continue to run on the CPU.		
Rationale: Design Requirement, need to ensure that users can continue to use GEANT-4 as before.		
Fit Criterion: Running an existing simulation should execute on the CPU by default as before with no performance regressions and identical results.		
Priority: High	History: Created September 29, 2015	

Req. #: 4	Req. Type: 4.4	Use Case #: 1
<p>Description: Trying to run the simulation on the GPU with a computer that does not have a compatible graphics card should be detected and cause it to run on CPU like before.</p> <p>Rationale: New product should not limit the amount of users who can use GEANT-4</p> <p>Fit Criterion: Any computer that can currently run the existing product should be able to run the new product.</p> <p>Priority: Medium</p> <p>History: Created September 29, 2015</p>		

5 Non-functional Requirements

5.1 Look and Feel Requirements

5.2 Usability and Humanity Requirements

First and foremost, it should be noted that the software-as-is (GEANT4) has an exceptionally high knowledge requirement. There is a lot assumed about the abilities of GEANT4 users in order for the software to be used successfully. Some, but not all, of these abilities may pertain to:

- Thorough understanding of quantum mechanics
- anticipated comfort in advanced algebras
- ability to construct GEANT4 geometry
- cognizance of and comfort with GEANT4 input file structure

5.2.a Ease of Use Requirements

The product shall expect no more in ability of the user than GEANT4 does already. It should be easy to use for a undergraduate student (or higher) of the physical sciences or nuclear/physical sciences who has already been

trained to use GEANT4.

5.2.b Personalization and Internationalization Requirements

The software will be adjustable given technical constraints of the user, according to GPU specifics. The product will not, however, be adjustable in terms of personal or national preferences. This processes involved in the software are in accordance with a strict scientific standard.

5.2.c Learning Requirements

Though the average user of GEANT4 should have the prerequisite knowledge of an undergrad (or even graduate) university student or researcher, the learning curve expected for these users is relatively low. With that said, it is still technical software and does require training. The training time for someone who has the requisite knowledge is roughly 3 weeks.

5.2.d Understandability and Politeness Requirements

Users of the product are expected to understand what the product will do for them and the analytics it offers into the problems they are trying to have.

5.2.e Accessibility Requirements

There will not be specific accessibility constraints placed with respect to the product. Any person with the ability to perform adequately in the academic setting, and with the ability to use shell based computers, will not have a problem with the software.

5.3 Performance Requirements

5.3.a Speed and Latency Requirements

Req. #: 5	Req. Type: 5.3	Use Case #: 1
Description: Decrease the time it takes to run a particle simulation while mainting the same output.		
Rationale: The entire purpose of the project is to improve the speed of the simulation.		
Fit Criterion: Running a simulation with a given set of input parameters should complete significantly faster on the product as compared to the existing software. Both should have identical outputs.		
Priority: Very High		History: Created September 27, 2015

5.3.b Safety Critical Requirements

NA

5.3.c Precision of Accuracy Requirements

Req. #: 6	Req. Type: 5.3	Use Case #: 1
Description: Results should have same accuracy whether simulation is run on CPU or GPU.		
Rationale: If results are not as accurate as with the existing product then researchers will not be able to draw as strong conclusions.		
Fit Criterion: The results of a simulation should be identical on the new product as the existing one, given that the inputs are the same.		
Priority: High		History: Created September 27, 2015

5.3.d Reliability and Availability Requirements

Req. #: 7	Req. Type: 5.3	Use Case #: 1
Description: The product should be at least as stable as the existing product.		
Rationale: Researchers require an extremely stable product, we do not want to introduce any new crashes or bugs.		
Fit Criterion: Testing the product with a variety of simulations should never result in a crash.		
Priority: High	History: Created September 27, 2015	

5.3.e Robustness or Fault-Tolerance Requirements

Req. #: 8	Req. Type: 5.3	Use Case #: 1
Description: .		
Rationale: .		
Fit Criterion: .		
Priority: High	History: Created September 27, 2015	

5.3.f Capacity Requirements

Req. #: 9	Req. Type: 5.3	Use Case #: 1
Description: Due to speed improvements (requirement 5) a larger number of particles should be able to be simulated in the same period of time.		
Rationale: Increasing the number of particles in the simulation will allow researchers to better simulate real-world interactions.		
Fit Criterion: A simulation running on the new product will be able to simulate a significantly larger number of particles in the same time as the same simulation on the existing product.		
Priority: High	History: Created September 27, 2015	

5.3.g Scalability Requirements

NA

5.3.h Longevity Requirements

NA

5.4 Operational and Environmental Requirements

5.4.a Expected Physical Environment

Req. #: 10	Req. Type: 5.4	Use Case #: 1
Description: The product shall be used by and engineering physics professor, researcher or student who will be sitting down in a temperature controlled environment.		
Rationale: The product should typically only be used in an office environment.		
Fit Criterion: 95% of all uses of the product will be used by engineering physics professors, researchers or students in sitting down in temperature controlled environments.		
Priority: High		History: Created October 4, 2015

5.4.b Requirements for interfacing with adjacent Systems

Req. #: 11	Req. Type: 5.4	Use Case #: 1
Description: The product shall work with the last four versions of GEANT4		
Rationale: Backwards compatibility is a nice thing to have.		
Fit Criterion: At least the last four versions of GEANT4 will be able to run this product.		
Priority: Low		History: Created October 4, 2015

5.4.c Productization Requirements

Req. #: 12	Req. Type: 5.4	Use Case #: 1
Description: The product will shall be distributed as a ZIP file, available on a public repository for users to download.		
Rationale: Want to make the product easily available for users to get		
Fit Criterion: 90% of users should be able to acquire the product with out much trouble		
Priority: Low	History: Created October 4, 2015	

5.4.d Release Requirements

Req. #: 13	Req. Type: 5.4	Use Case #: 1
Description: Later versions of the product that have been patch will be available on the public repository. Each release shall not cause previous features to fail		
Rationale: If the product needs to be patched, it should not break older features. It should also be available in the same location as where the product is acquired		
Fit Criterion: Upon patching the product, none of the previous features should fail.		
Priority: Medium	History: Created October 4, 2015	

5.5 Maintainability and Support Requirements

5.6 Security Requirements

5.6.a Access Requirements

All users have access to all parts of the product, as the product will be open-source.

5.6.b Integrity Requirements

All data is stored and manipulated locally. Because of this, there will be no compromise on the integrity of data outside of physical hardware malfunctions.

5.6.c Privacy Requirements

All data is stored and manipulated locally. Because of this, the privacy of said data is entirely at the discretion of the user. With that said, there will also be no local encryption on the output and input files used for the software.

5.6.d Audit Requirements

NA

5.6.e Immunity Requirements

The only aspect of the project at risk with respect to external software is performance. The user is held responsible for ensuring that no external software is hogging the resources required for the project to run at optimal performance.

5.7 Cultural Requirements

NA

5.8 Legal Requirements

5.8.a Compliance Requirements

NA

5.8.b Standards Requirements

NA

6 Project Issues

6.1 Open Issues

6.2 Off-the-Shelf Solutions

6.3 New Problems

6.3.a Effects on the Current Environment

The new product will be designed as an opt-in addition to the existing product. That is, unless manually changed by the user, the program will execute identically as before, running on the CPU. The motivation for this is to ensure compatibility, as the programming environment for GPGPU programming is restricted to certain hardware. The current environment will not be affected by the changes unless the user specifically decides to use them.

6.3.b Effects on the Installed Systems

Requirement 2 specifies the importance of creating a simple interface for the user to enable the changes in the new system, or revert to the previous one. Changes to the code will be isolated, and only used when they are manually enabled.

6.3.c Potential User Problems

Due to the separation of the changes and the existing product, users will not negatively respond to the changes, indeed they won't even notice them unless actively looking. To use the new product's features, users will enable them

and then execute the program in an identical manner to how the existing software works (requirement 2).

6.3.d Limitations of the Anticipated Implementation Environment That May Inhibit the New Product

To run the GPGPU computations, specific hardware is required (recent NVIDIA graphics card).

6.3.e Follow-Up Problems

There are a number of potential situations that could lead to the product failing. We are confident that we will be able to succeed, however we realize that there is a possibility of failure, and have outlined the potential causes below.

- Learning curve for existing GEANT-4 codebase is too steep, cannot gain adequate understanding to implement changes in time constraints
- Porting existing algorithms to CUDA requires too much work, and we are not able to run the algorithms on a GPU within time constraints
- The current product's interface for the specific algorithms that will be ported is not well-enough defined
- The large models used in the simulation exceed memory limitations on the GPU, and cannot be run on existing hardware
- Performance gains from the GPU are negligible, due to the structure of the computations
- Numerical accuracy problems lead to different results from simulations run on the existing product vs. the new product

6.4 Tasks

Record of Proposed Project	September 18
Problem Statement	September 25
Requirements Document Revision 0	October 9
Proof of Concept Plan	October 23

Test Plan Revision 0	October 30
Proof of Concept Demonstration	November 16 - 27
Design Document Revision 0	January 1
Revision 0 Demonstration	February 1 - 27
User's Guide Revision 0	February 29
Test Report Revision 0	March 21
Final Demonstration (Revision 1)	Exam period
Final Documentation (Revision 1)	April 1

6.5 Migration to the New Product

6.6 Risks

6.7 Costs

All software used in the project is open-source and/or available for free. Existing hardware will be used for development, so there are no associated monetary costs.

We have very clear and well-defined deadlines for each deliverable, and are in full confidence that we will meet each one. The time it takes for each deliverable will be variable, but the date of completion for each is concrete, as outlined in 6.4.

6.8 User Documentation and Training

- Function descriptions shall be provided for every new function in the code
- There shall be a thorough Read Me file accompanying the project that will explain to the user the changes as well as how to use the new functions
- Users who know how to use GEANT4 should be able to easily use the new functions

6.9 Waiting Room

6.10 Ideas for Solutions