

# 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	2015-10-07

## 2 Project Drivers

### 2.1 Purpose of Project

#### 2.1.a Project Background

Physics researchers use software simulations to model how particles interact with environments, and to determine the effects of these interactions. Members of McMaster’s Engineering Physics department use GEANT-4 – a simulation toolkit developed by CERN. McMaster’s researchers have developed their own fork of the software, G4-STORK, designed to study McMaster’s nuclear reactor. Currently, running G4-STORK simulations (as well as other GEANT-4 simulations) that require many particle takes a long time to compute when run on the CPU. This limits researchers to smaller number of particles than are realistic, and prevents them from seeing the effects of longer time periods.

#### 2.1.b Goal of the project

The goal of this project is to significantly increase the computation speed of G4-STORK simulations, which should transfer well to other GEANT-4 projects. Increasing the speed will allow researchers to use more accurate models, to see the effects of longer time periods on the particles, and to generally increase their productivity. This will be achieved by porting the algorithms that currently run on the CPU to the GPU, taking advantage of the parallel power of the GPU’s many cores.

### 2.2 Stakeholders

The stakeholders that are currently involved with the project are:

- the project group
- the supervisors of the project (Dr. Adriaan Buijs and Dr. Emil Sekerenski)
- McMaster Engineering Physics Department, specifically grad student Wesley Holbrook

### **2.2.a The Client**

The clients for the project are the Dr. Buijs and his grad student Wesley Holbrook, representing the McMaster Engineering Physics Department. The clients proposed the project because they have invested interest in running G4-STORK simulations more efficiently. They will be using the parallelized code to run and study nuclear simulations, and require that the code executes much more quickly to obtain useful data.

### **2.2.b The Customer**

The customer in this case also includes the clients. 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 GEANT-4 users external to McMaster could be potential stakeholders. If the software is successfully completed and the resulting performance improvements are significant, the changes will be submitted to the GEANT-4 repository. It is then up to the GEANT-4 group to decide if those contributions are accepted or not, and if they are then all users of GEANT-4 stand to benefit from them. However, they are not considered stakeholders throughout the development of the project, the focus is instead on those mentioned in 2.2.

#### **2.2.d The Hands-On Users of the Product**

Graduate students and professors from the McMaster Engineering Physics Department will be hands-on users of the product. They will all have familiarity with the existing product.

#### **2.2.e Personas**

Consider Matt Douglas, a graduate student in the Engineering Physics Department. Matt wants to study how particles in McMaster's nuclear reactor affect each other, given some specific starting conditions, and a very large number of particles. Matt knows how to use the existing G4-STORK program, but it will take weeks to run the computations. Matt inputs his desired number of particles and specific starting conditions into a G4-STORK simulation. He enables the GPU features of the new product, and successfully runs the simulation in a reasonable amount of time. He observes interesting results that would not have been feasible to obtain with the old product.

#### **2.2.f Priorities Assigned to Users**

Priority will be given to Wesley Holbrook, the grad student that proposed the project to Dr. Buijs. He will be the primary user of G4-STORK as it is integral to his current research.

### **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 GEANT-4 code, which is used by G4-STORK to run the simulation. The final product must be able to run any code/simulation that ran on the existing software. The software must run in parallel on a 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.

Table 2: Glossary

Term	Description
GEANT-4	open-source software toolkit used to simulate the passage of particles through matter
G4-STORK	(Geant-4 STOchastic Reactor Kinetics), fork of GEANT-4 developed by McMaster’s Engineering Physics department to simulate McMaster’s nuclear reactor
GPU	graphics processing unit, well-suited to parallel computing tasks
CPU	computer processing unit, general computer processor well-suited to serial tasks
GP-GPU	concept of running “general-purpose” computations on the GPU
CUDA	parallel computing architecture for general purpose programming on GPU, developed by NVIDIA

## 3.3 Relevant Facts and Assumptions

### 3.3.a Facts

- GEANT-4/G4-STORK are programmed in C++
- GEANT-4/G4-STORK run simulations on the CPU
- Simulations run calculations on each particle independently
- 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 G4-STORK

## 4 Functional Requirements

### 4.1 The Scope of the Work

#### 4.1.a The Current Situation

The project, G4-STORK, is currently at a point where it is able to run all necessary simulations, on the CPU. The time to run these simulations is significant.

#### 4.1.b The Context of The Work

#### 4.1.c Work Partitioning

#### 4.1.d Specifying a Business Use Case (BUC)

### 4.2 Business Data Model & Data Dictionary

NA – The product does not store any data, and requires no data model.

### 4.3 The Scope of the Product

The following table outlines the use cases for the product.

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)

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

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 traveled, so researchers can study where the particles are most probably to end up.

## 4.4 Functional Requirements

<b>Req. #:</b> 1	<b>Req. Type:</b> 4.4	<b>Use Case #:</b> 1
<b>Description:</b> Particle computations run on the GPU		
<b>Rationale:</b> Design requirement, will allow particle simulations to run faster (requirement 6)		
<b>Fit Criterion:</b> 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)		
<b>Priority:</b> Very High	<b>History:</b> Created September 29, 2015	

  

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

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

<b>Req. #:</b> 4	<b>Req. Type:</b> 4.4	<b>Use Case #:</b> 1
<p><b>Description:</b> 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><b>Rationale:</b> New product should not limit the amount of users who can use GEANT-4</p> <p><b>Fit Criterion:</b> Any computer that can currently run the existing product should be able to run the new product.</p> <p><b>Priority:</b> Medium</p>		
		<b>History:</b> Created September 29, 2015

## 5 Non-functional Requirements

### 5.1 Look and Feel Requirements

#### 5.1.a Appearance Requirements

NA – The scope of the project does not include any visual aspects. Simulations are run through the command line.

### 5.1.b Style Requirements

<b>Req. #:</b> 5	<b>Req. Type:</b> 5.1	<b>Use Case #:</b> 1
<b>Description:</b> The code should be well organized and appear readable to any who might want to edit it.		
<b>Rationale:</b> Revised code should not inhibit the modifying or understanding of G4-STORK		
<b>Fit Criterion:</b> Any persons with an understanding of the existing project should be able to clearly understand the modified code.		
<b>Priority:</b> Medium		<b>History:</b> Created October 6, 2015

## 5.2 Usability and Humanity Requirements

## 5.3 Performance Requirements

### 5.3.a Speed and Latency Requirements

<b>Req. #:</b> 6	<b>Req. Type:</b> 5.3	<b>Use Case #:</b> 1
<b>Description:</b> Decrease the time it takes to run a particle simulation while maintaining the same output.		
<b>Rationale:</b> The entire purpose of the project is to improve the speed of the simulation.		
<b>Fit Criterion:</b> 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.		
<b>Priority:</b> Very High		<b>History:</b> Created September 27, 2015

### 5.3.b Safety Critical Requirements

NA – The software is not used in safety critical environments. It is a tool for researchers to study particle interactions.

### 5.3.c Precision of Accuracy Requirements

<b>Req. #:</b> 7	<b>Req. Type:</b> 5.3	<b>Use Case #:</b> 1
<b>Description:</b> Results should have same accuracy whether simulation is run on CPU or GPU.		
<b>Rationale:</b> If results are not as accurate as with the existing product then researchers will not be able to draw as strong conclusions.		
<b>Fit Criterion:</b> The results of a simulation should be identical on the new product as the existing one, given that the inputs are the same.		
<b>Priority:</b> High	<b>History:</b> Created September 27, 2015	

### 5.3.d Reliability and Availability Requirements

<b>Req. #:</b> 8	<b>Req. Type:</b> 5.3	<b>Use Case #:</b> 1
<b>Description:</b> The product should be at least as stable as the existing product.		
<b>Rationale:</b> Researchers require an extremely stable product, we do not want to introduce any new crashes or bugs.		
<b>Fit Criterion:</b> Testing the product with a variety of simulations should never result in a crash.		
<b>Priority:</b> High	<b>History:</b> Created September 27, 2015	

### 5.3.e Robustness or Fault-Tolerance Requirements

NA – The product does not need to maintain standards during an unforeseen event. It does not handle any sensitive data, and is not constantly required to be running by its users.

### 5.3.f Capacity Requirements

<b>Req. #:</b> 9	<b>Req. Type:</b> 5.3	<b>Use Case #:</b> 1
<b>Description:</b> Due to speed improvements (requirement 6) a larger number of particles should be able to be simulated in the same period of time.		
<b>Rationale:</b> Increasing the number of particles in the simulation will allow researchers to better simulate real-world interactions.		
<b>Fit Criterion:</b> 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.		
<b>Priority:</b> High		<b>History:</b> Created September 27, 2015

### 5.3.g Scalability Requirements

NA – The product will be used by single researchers, and is run locally on their machines.

### 5.3.h Longevity Requirements

NA – The product is to be completed by April 2016, and there are no plans to extend that lifetime.

## 5.4 Operational and Environmental Requirements

### 5.4.a Expected Physical Environment

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

### 5.4.b Requirements for interfacing with adjacent Systems

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

#### 5.4.c Productization Requirements

<b>Req. #:</b> 12	<b>Req. Type:</b> 5.4	<b>Use Case #:</b> 1
<b>Description:</b> The product will available on a public repository along with clear instructions for installation		
<b>Rationale:</b> Want to make the product easily available		
<b>Fit Criterion:</b> 90% of users should be able to acquire the product with out much trouble		
<b>Priority:</b> Low		<b>History:</b> Created October 4, 2015

#### 5.4.d Release Requirements

<b>Req. #:</b> 13	<b>Req. Type:</b> 5.4	<b>Use Case #:</b> 1
<b>Description:</b> New versions of the product that have been patched will be available on the public repository and shall not cause previous features to fail.		
<b>Rationale:</b> Users should be encouraged to use the latest patch, and should be confident that updating won't negatively impact their work		
<b>Fit Criterion:</b> Each new patch of the product will not cause any previous features to fail.		
<b>Priority:</b> Medium		<b>History:</b> 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 aspects 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 – The product does not store any persistent information.

### **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 – The product is intended for a small number of stakeholders. All content is objective and scientific.

## **5.8 Legal Requirements**

### **5.8.a Compliance Requirements**

NA – The product does not store or access any user information. It does not need to comply with any legal standards.

### **5.8.b Standards Requirements**

NA – There are no internal standards that are required to be met by the product.

## **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 GP-GPU 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 GP-GPU 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 G4-STORK 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 Readme file accompanying the project that will explain to the user the changes as well as how to enable GPU computation
- Users who know how to use G4-STORK should be able to easily run it on the GPU

## **6.9 Waiting Room**

## **6.10 Ideas for Solutions**