

GEANT-4 GPU Port:

Design Document: Detailed Design

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1 Introduction

1.1 Revision History

All major edits to this document will be recorded in the table below.

Table 1: Revision History

Description of Changes	Author	Date
Set up sections and filled out Introduction section	Matthew	2015-12-15
Added sections for Errors and Key Algorithms	Stuart	2016-01-08

1.2 Document Structure & Template

The design documentation for the project is broken into two main documents.

The system architecture document details the system architecture, including an overview of the modules that make up the system, analysis of aspects that are likely and unlikely to change, reasoning behind the high-level decisions, and a table showing how each requirement is addressed in the proposed design.

This detailed design document covers the specifics of several key modules in the project. For each module, an MIS is given fully detailing the interface of the module. Then, the methods for handling errors within the module are discussed, and finally the main algorithms and data structures used by the module are presented.

1.3 List of Tables

Table #	Title
1	Revision History
2	G4NeutronHPDataPoint – access program syntax
3	G4NeutronHPDataPoint – access program semantics
7	G4NeutronHPDataPoint – state variables
5	G4NeutronHPVector – access program syntax
6	G4NeutronHPVector – access program semantics
7	G4NeutronHPVector – state variables
8	CMake Files – state variables

1.4 Technologies and Languages

Geant4 is developed entirely in C++. The project will use C++ as the interface between the GPU code and the existing Geant4 codebase. All GPU code will use

CUDA, as discussed in the system architecture document. Other technologies used are CMake for the build system (see section 4.1).

1.5 Notes

Geant4 uses its own basic types for standard C++ types (G4int, G4bool, G4double, etc). These types are currently just **typedefs** to the respective type as defined in the system libraries.

The modules G4NeutronHPDataPoint and G4NeutronHPVector described below are existing modules of Geant4. All methods and state variables are pre-existing, and will be replicated on the GPU. The interface of the modules will not change.

2 G4NeutronHPDataPoint

2.1 Description

This class encapsulates all of the data as well as the setter and getter methods that each data point in G4NeutronHPVector's list of data requires. Two private variables are used to store the xSection and the energy of the data point.

2.2 MIS (Module Interface Specification)

2.2.1 Access Program Syntax

Table 2: G4NeutronHPDataPoint – access program syntax

Routine Name	Input	Output	Exceptions
G4NeutronHPDataPoint			
G4NeutronHPDataPoint	G4double, G4double		
=	G4NeutronHPDataPoint		
GetEnergy		G4double	
GetXsection		G4double	
SetEnergy	G4double		
SetXsection	G4double		
GetX		G4double	
GetY		G4double	
SetX	G4double		
SetY	G4double		
SetData	G4double, G4double		

2.2.2 Access Program Semantics

Note that hyphens in routine names and inputs are just for line breaks due to the table size. The actual routine names and inputs do not have hyphens.

Table 3: NeutronHPDataPoint – access program semantics

Routine Name	Input	Semantics
G4NeutronHPDataPoint		instantiates the class, setting energy and xSec to 0
G4NeutronHPDataPoint	G4double, G4double	instantiates the class with the inputted energy and xSec
=	G4NeutronHP- DataPoint	sets the energy and xSec of the instance to those of the input
GetEnergy		returns energy of the instance
GetXsection		returns the xSec of the instance
SetEnergy	G4double	sets energy of instance to the argument
SetXsection	G4double	sets xSec of instance to the argument
GetX		returns the energy of the instance
GetY		returns the xSec of the instance
SetX	G4double	sets energy of instance to the argument
SetY	G4double	sets xSec of instance to the argument
SetData	G4double, G4double	sets instance's energy and xSec to the passed arguments

2.2.3 State Variables

The following variables maintain state for the class, and are all private to the module.

Table 4: G4NeutronHPDataPoint – state variables

Variable	Type	Description
energy	G4double	the energy of the particle
xSec	G4double	the cross-section of the particle

2.2.4 Environment Variables

There are no environment variables for this module.

2.2.5 Assumptions

It can be assumed that the class will be initialized. As such, all getter methods will return a non-null value.

2.3 Error Handling

This module does not handle errors explicitly.

2.4 Key Algorithms

This module represents data, and as such does not contain any algorithms.

3 G4NeutronHPVector

3.1 Description

This module stores a large vector of data points (G4NeutronHPDataPoint). It includes functions for setting the data points, retrieving them, and calculating information over them (such as the integral).

3.2 MIS (Module Interface Specification)

Note that hyphens in routine names, inputs, outputs, and exceptions are just for line-breaks due to the table size. The actual routine names, inputs, outputs, and exceptions do not have hyphens.

3.2.1 Access Program Syntax

Table 5: G4NeutronHPVector – access program syntax

Routine Name	Input	Output	Exceptions
G4NeutronHPVector			
G4NeutronHPVector	G4int		
=	G4NeutronHPVector&	G4NeutronHPVector&	
+	G4NeutronHPVector&, G4NeutronHPVector&	G4NeutronHPVector&	
SetVerbose	G4int		
Times	G4double		
SetPoint	G4int, G4NeutronHPDataPoint		
SetData	G4int, G4double, G4double		
SetX	G4int, G4double		
SetEnergy	G4int, G4double		
SetY	G4int, G4double		
SetXsec	G4int, G4double		

GetEnergy	G4int	G4double
GetXsec	G4int	G4double
GetXsec	G4double	G4double
GetXsec	G4double,G4int	G4double
GetX	G4int	G4double
GetY	G4double	G4double
GetY	G4int	G4double
GetVectorLength		G4int
GetPoint	G4int	const G4NeutronHPDataPoint&
Hash		
ReHash		
InitInterpolation	istream	
Init	istream,G4int, G4double, G4double	
Init	istream, G4double,G4double	
ThinOut	G4double	
SetLabel	G4double	
GetLabel		G4double
CleanUp		
Sample		G4double
Debug		G4double *
Merge	G4NeutronHPVector *, G4NeutronHPVector *	
Merge	G4InterpolationScheme, G4double, G4NeutronHPVector *, G4NeutronHPVector *	
SampleLin		G4double
IntegrateAndNormalise		
Integrate		
GetIntegral		G4double
SetInterpolationManager	const G4InterpolationManager &	
SetInterpolationManager	G4InterpolationManager &	
SetScheme	G4int,const G4InterpolationScheme &	

GetScheme	G4int	G4InterpolationScheme	
GetMeanX		G4double	
GetBlocked		vector<G4double>	
GetBuffered		vector<G4double>	
Get15percentBorder		G4double	
Get50percentBorder		G4double	
Check	G4int		G4Hadronic- Exception

3.2.2 Access Program Semantics

Note that hyphens in routine names and inputs are just for linebreaks due to the table size. The actual routine names and inputs do not have hyphens.

Table 6: G4NeutronHPVector – access program semantics

Routine Name	Input	Description
G4NeutronHPVector		Instantiates the class with no parameters
G4NeutronHPVector	G4int	Instantiates the class with the number of points to consider as the parameter
=	G4NeutronHPVector&	Sets the current instance to the passed instance
+	G4NeutronHPVector&, G4NeutronHPVector&	Returns the vector addition of the two passed vectors
SetVerbose	G4int	sets the verbosity to the input
Times	G4double	Multiplies all points y-values and integrals from theData by the input
SetPoint	G4int, G4NeutronHP-DataPoint	sets point at passed index to the passed point
SetData	G4int, G4double, G4double	sets point at passed index with given values
SetX	G4int, G4double	sets x value of point at passed index to passed value
SetEnergy	G4int, G4double	sets x value of point at passed index to passed value
SetY	G4int, G4double	sets y value of point at passed index to passed value
SetXsec	G4int, G4double	sets y value of point at passed index to passed value
GetEnergy	G4int	returns x value of point at passed index
GetXsec	G4int	returns y value of point at passed index

GetXsec	G4double	returns y value of point with lowest xSection above passed double
GetX	G4int	returns x value of point at passed index
GetY	G4int	returns y value of point at passed index
GetVectorLength		returns number of points
GetPoint	G4int	returns point at passed index
Hash		sets theHash 's up based on theData
ReHash		clears theHash and re-evaluates it based on theData
InitInterpolation	istream	sends the passed data file to the interpolation manager
Init	istream, G4int, G4double, G4double	initializes class and theHash
Init	istream, G4double, G4double	initializes class and theHash
ThinOut	G4double	removes unnecessary points and rehashes
SetLabel	G4double	sets the label value to passed number
GetLabel		returns the label of the current instance
CleanUp		clears all data
Sample		performs samples of X according to interpolation scheme
Debug		returns theIntegral
Merge	G4NeutronHPVector*, G4NeutronHPVector*	interpolate between labels, continue in unknown areas by subtraction of the last difference
Merge	G4InterpolationScheme, G4double, G4NeutronHPVector*, G4NeutronHPVector*	interpolate between labels according to passed G4InterpolationScheme, cut at passed G4double, continue in unknown areas by subtraction of the last difference.
SampleLin		samples X according to distribution Y, linear
IntegrateAndNormalise		calculates the integral for every data point and normalizes each
Integrate		calculates the integral for every data point
GetIntegral		linearly interpolates over theIntegral
SetInterpolation-Manager	G4Interpolation-Manager&	sets theManager to the input
SetScheme	G4int, G4InterpolationScheme&	appends the passed G4InterpolationScheme to theManager
GetScheme	G4int	returns the current G4InterpolationScheme associated with theManager

GetMeanX		returns the average x value of all data points
GetBlocked		returns the current value of theBlocked
GetBuffered		returns the current value of theBuffered
Get15percentBorder		gets the integral from each data point to the last data point and returns the first one within 15% of the last data point
Get50percentBorder		gets the integral from each data point to the last data point and returns the first one within 50% of the last data point
Check	G4int	checks that passed index is greater than the number of points, throwing an exception if not

3.2.3 State Variables

The following variables maintain state for the class, and are all private to the class. Note that hyphens in variable names and types are just for line breaks due to the table size. The actual variable names and types do not have hyphens.

Table 7: G4NeutronHPVector – state variables

Variable	Type	Description
theLin	G4NeutronHP-Interpolator	the linear interpolator for sampling data
totalIntegral	G4double	integral over all data points from theData
theData	G4NeutronHP-DataPoint*	array of G4NeutronHPDataPoint, stores all data points in vector
theManager	G4Interpolation-Manager	manages the interpolation schemes, knows how to interpolate data
theIntegral	G4double*	array of integrals where theIntegral[i] is the integral of all data points from theData up until <i>i</i>
nEntries	G4int	the number of data points to consider when performing calculations over theData
nPoints	G4int	the number of data points in theData
label	G4double	number tagging class instance
theInt	G4Neutron-Interpolator	the interpolator for sampling data (may not be linear)
Verbose	G4int	verbosity level, some statements will only print to console with higher values
isFreed	G4int	only used for debugging, 1 if class has been destructed 0 otherwise
theHash	G4NeutronHP-Hash	stores the <i>x</i> and <i>y</i> value of every tenth data point from theData to speed up getting the minimum index in theData of a data point with X larger than a given value
maxValue	G4double	maximum value of Xsec or Y passed in SetData, SetY, or SetXSec so far. Initialized to -DBL_MAX (min representable double).
theBlocked	vector <G4double>	deprecated: vector still exists in class but data never added to it
theBuffered	vector <G4double>	stores buffer of samples to speed up sampling the vector
the15percent-BorderCash	G4double	the X value of the first data point with an integral no more than 15% smaller than the integral of the last data point
the50percent-BorderCash	G4double	the X value of the first data point with an integral no more than 50% smaller than the integral of the last data point

3.2.4 Environment Variables

There are no environment variables for this module.

3.2.5 Assumptions

It can be assumed that the module will be initialized before other functions are called.

3.3 Error Handling

The `Check` method throws a `G4HadronicException` on error, however it is the only function to do so in the module. In the other functions, erroneous input is not handled explicitly beyond control statement checks that will assume default values for any invalid parameters.

3.4 Key Algorithms

There are a variety of algorithms used in the module. When porting to the GPU, the same algorithms will be modified to run in parallel. In general, this consists of taking array traversals and running the procedures executed sequentially at the same time on different cores of the GPU.

4 CMake Files

4.1 Description

The current build system used by Geant4 is CMake, consisting of *CMakeLists* text files in each source code directory detailing the files to compile and link, and further compiler directives. The user calls the `cmake` program with arguments (such as *useCuda*) for the build to generate the necessary makefiles. Support for CUDA and the *nvcc* CUDA compiler are built in to CMake. Although not a module in the traditional sense, CMake will still be the basis for enabling and disabling GPU functionality, and was included for that reason.

4.2 MIS (Module Interface Specification)

4.2.1 Access Program Syntax

CUDA support is built in to CMake, as such no new access programs or public macros will be created.

4.2.2 Access Program Semantics

CUDA support is built in to CMake, as such no new access programs or public macros will be created.

4.2.3 State Variables

Table 8: CMake Files – state variables

Variable	Type	Description
useCuda	Boolean	if set to true, the makefiles generated by CMake will include directives to compile and link the CUDA code and will execute ported procedures on the GPU. Default is false.

4.2.4 Environment Variables

- CUDA source files (.cu) containing the GPU code. CMake files will contain directives to compile and link the CUDA files.
- Source code from Geant4 project, such as the G4NeutronHPVector.cpp file. The relevant source code files will be compiled and linked as per CMake directives to the CUDA files listed above.

4.2.5 Assumptions

It is assumed the user has CMake installed, as it is required for Geant4.

4.3 Error Handling

If the tries to enable CUDA without compatible hardware, CMake will detect this and output a fatal error message. The user will not be able to enable CUDA unless they have compatible hardware. If the user is using an older version of CMake (before 2.8) that does not support CUDA compilation, a fatal error message will be outputted.

4.4 Key Algorithms

CMake is the existing build system for generating make files for the project. As such, there are no key algorithms to document.