Transforming Geant4 for the Future

Bob Lucas and Rob Roser
USC and FNAL
May 8, 2012

Welcome

Associate Directors of Science

Dan Hitchcock	**Advanced Scientific Computing Research**
Jim Siegrist	**High Energy Physics**

Program Managers

Ceren Susut	**Advanced Scientific Computing Research**
Lali Chatterjee	**High Energy Physics**

Workshop Chairs

Bob Lucas	**University of Southern California**
Rob Roser	**Fermi National Accelerator Center**

Oak Ridge Institute for Science and Education

Donna Nevels

Scientific Challenge

Addressing challenges related to big data is a national priority

High Energy Physics experiments generate vast amounts of data

Geant4 is used to design the experiments, their data handling infrastructure, and the analysis of the data

Geant4 is essential to the success of HEP but is of great interest to other fields as well – our success here will ultimately benefit many scientific endeavors

Geant4 must scale to support the physics modeling needs of future HEP experiments

Direction from DOE

Department of Energy
Office of Science
Washington, DC 20585

March 7, 2012

Dr. Robert F. Lucas
Information Sciences Institute
University of Southern California
4676 Admiralty Way, Suite 1001
Marina Del Rey, CA 90292

Dr. Robert M. Roser
Particle Physics Division
Fermi National Laboratory
Wilson and Kirk Roads
Mail Station: 318 (CDF ASSY HALL)
Batavia, IL 60510-5011

Dear Drs. Lucas and Roser:

Thank you for agreeing to organize and co-chair a workshop on issues related to, "Transforming Geant4 for the Future."

The Department of Energy's (DOE) Office of High Energy Physics (HEP) and Office of Advanced Scientific Computing Research (ASCR) are co-sponsoring this workshop to identify opportunities and needs for leveraging the powerful physics capabilities of Geant4 into a robust, sustainable software infrastructure. This workshop will identify applied mathematics, computer science and algorithm development challenges in effectively transitioning Geant4 to new computer architectures. This workshop will examine opportunities for discovery enabled by numerical algorithms and optimization tools likely to emerge from current ASCR investments to meet these challenges. This workshop will explore models of collaborative efforts that include applied mathematicians, computer scientists, algorithm developers as well as Geant4 users to optimize productivity and the scientific advances through modeling and simulation. The workshop has the opportunity to influence future HEP and ASCR investment decisions.

The goals of this workshop are to:

- Identify and review the current status, successes and limitations of the Geant4 software toolkit including the international scene;
- Determine the challenges that lie ahead in transforming Geant4 into a software that runs effectively in new architectures;
- Consider the opportunities related to existing algorithms, optimization tools and physics models;
- Ascertain research areas in applied mathematics, computer science, algorithm development and simulation strategies needed to leverage the powerful physics capabilities of Geant4 into a robust, sustainable software infrastructure;
- Create the foundation for information exchanges and collaborations among ASCR and HEP supported researchers, ASCR computing facilities and Geant4 user community;
- Understand the research that may currently be in progress at the international level and identify directions that would not duplicate existing projects;
- Explore possibilities for transformative advances that could ensue through the unique characteristics of the HEP-ASCR collaborations.

The workshop should focus on areas of research and collaboration to position Geant4 to exploit emerging computer architectures, while providing for a strong, diverse and potentially changing user community. We anticipate that the workshop will develop findings in the context of HEP and ASCR missions and the collaborative exchanges between the two communities will seed fruitful directions that enhance the impact of the workshop. We anticipate that you will establish a program committee to organize the workshop and that the workshop will consist of plenary and breakout sessions.

The workshop should be held in the Washington, DC, metropolitan area in early to mid-May 2012 time frame. We request that a written report representing the results of the workshop be prepared by you as workshop chairs, with inputs from panel leads, and other assigned writers. The report should specifically address all workshop goals. We would like a draft version of the Executive Summary, containing an overview of the major findings of the workshop, within 45 days after the workshop. The final report will be used by HEP and ASCR to shape out-year program plans and to inform the Office of Science long-range budget planning process.

Dr. Ceren Susut (Ceren.Susut-Bennett@science.doe.gov), ASCR, and Dr. Lali Chatterjee (Lali.Chatterjee@science.doe.gov), HEP, will be your primary DOE contacts for this workshop and will provide any support needed to organize and conduct a successful workshop.

This workshop is an important step toward developing and executing the strategic vision for porting Geant4 in the future through a partnership between HEP and ASCR. Thank you again for agreeing to contribute to this effort.

Sincerely,

Dr. Daniel A. Hitchcock
Associate Director of Science for the
Office of Advanced Scientific Computing

Dr. James Siegrist
Associate Director of Science for the
Office of High Energy Physics

Direction from DOE, cont.

Review the current status, success and limitations of Geant4

Determine the challenges posed by new processor architectures

Consider opportunities in algorithms, optimization tools, and physics models

Ascertain research areas needed to leverage Geant4 into a robust, sustainable software infrastructure

Create the foundation for collaboration between ASCR and HEP researchers, ASRC computing facilities, and Geant4 users

Understand current international research to avoid duplication

Explore transformative advances possible in a joint ASCR-HEP collaboration

May 8 Plenary Agenda

8:00-8:30 am	Registration Open	Continental Breakfast
8:30-9:00 am	Welcome and Goals	
	ASCR and HEP	Dan Hitchcock, ASCR
		Jim Siegrist, HEP
	Conference Chairs	Bob Lucas, USC
		Rob Roser, FNAL
9:00-9:30 am	Geant4 Overview	Amber Boehnlein, SLAC
9:30-9:45 am	Geant4 Collaboration and History	Makoto Asai, SLAC
9:45-10:15 am	Physics uses of Geant4	Tom LeCompte, ANL
10:15-10:45 am	Break	
10:45-11:15 am	Multi-core & Optimization	Rob Fowler, UNC
11:15-11:45 am	Exploiting Concurrency in Geant4	Jim Kowalkowski, FNAL
11:45-12:15 pm	Scientific Data Management	Rob Ross, ANL
12:15-12:30 pm	Charge to Workshop Participants	Bob Lucas, USC
		Rob Roser, FNAL
12:30-1:45 pm	Lunch on your own	

May 8 Breakout Agenda

1:45-3:15 pm	Parallel Sessions Multi-core Optimization Scientific Data Handling and Analysis
3:15-3:30 pm	Break
3:30-5:00 pm	Resume Sessions
5:00-5:30 pm	Report of Parallel Session progress
5:30 pm	Adjourn for the day

May 9 Agenda

8:00-8:30 am	Continental Breakfast
8:30-10:30 am	Resume breakout discussions
10:30-11:00 am	Break
11:00-12:00 pm	Plenary reports from discussions
12:00-12:15 pm	Closing remarks and paths forward
12:15-1:30 pm	Workshop adjourn
	Working lunch for organizers and chairs
1:30 pm	Report preparation

Break-out Objectives Include

Multi-core Optimization: Rob Fowler & Daniel Elvira

- Evolution of VLSI technology and the implications for Geant4
- Programming languages and code structure vs. the limits of optimizing compilers.
- Ideas on how to parallelize Geant4 for multicore processors
- Alternatives such as use of Domain Specific Languages

Scientific Data Handling and Analysis: Rob Ross & Gene Cooperman

- A few Topics to be covered in this session include:
- Geant4 as a way to leverage big data (test beds, prototyping etc)
- Strategies/Issues with generating very large simulations on GRIDS
- How to exploit new storage technologies that are on the horizon

Workshop Outcome

Our goal is to help DOE set its research agenda

- **This workshop could help shape HEP and ASCR out-year program plans**
- **It could also inform the Office of Science's long-range budget plans**

We will produce:

- **A briefing summarizing the workshop for DOE at 12:00 on Wednesday**
- **An executive summary delivered to DOE by June 23rd**
- **A white paper from the ASCR and HEP research communities which articulates the above and a puts forward a plan to succeed**
  - **Research agenda for big data problems typified by HEP**
  - **Research challenges for scaling Geant4 in multicore era**