



# Development of advanced features for the Geant4 simulation toolkit



Principal Investigator(s): M.Potekhin (**PO**)

List of the proposal participants and their organizations if other than NPP:

G. Galgoczi, A.Natochii (**EIC**), S.Rahman, D.Smirnov

ECA eligibility: A.Natochii

Proposal term from: 10/01/2026 to: 09/30/2028

Annual funding: FY27 \$250,000 FY28 \$250,000



# Project Description – goals and deliverables (1)

Geant4 is the preeminent simulation tool in Nuclear and Particle Physics experiments. Informed by our long experience in utilizing this tool in a variety of applications, we identified areas where improvements need to be made, which would result in both better efficiency and accuracy of computations. Below is the itemized list of goals and deliverables included in this proposal:

## 1. Enhanced scheduling logic and interface between GPU and CPU

Motivation	Suboptimal computational efficiency of Geant4 on heterogeneous platforms due to lack of runtime adaptive workload distribution between CPU and GPU, resulting in underutilized accelerator resources and load imbalance.
Goal	Develop a Geant4-native Task Scheduler with dynamic CPU/GPU workload partitioning based on runtime performance calibration, enabling non-blocking accelerator dispatch while maintaining compatibility with existing tasking infrastructure.
Deliverables and timeline	Geant4-native <i>Task Scheduler</i> leveraging the latest developments in the core Geant4. Functional prototype in FY27, inclusion in the Geant4 code base by end of FY28.
Personnel	G. Galgoczi, D.Smirnov

# Project Description – goals and deliverables (2)

2. Improvement of physics models used in Geant4 and leveraging parallelism for more efficient execution of X-ray dominated workloads.

Motivation	Standard X-ray reflection models supplied in Geant4 are not sufficient for efficient and accurate simulation of detector and accelerator components (cf IR of the EIC).
Goal	Create improved physics models for X-ray propagation, including diffuse reflection properly incorporating surface roughness.
Deliverables and timeline	Contribution of the enhanced models to the Geant4 code base, in two phases in FY27 and FY28
Personnel	A.Natochii

3. Application of AI to risk reduction when running expensive simulation workflows.

Motivation	Potential discrepancies between engineering design (CAD) and geometry used in Geant4 simulations (such as Geant4), with simulation errors as the result.
Goal	Create a tool for AI-driven diagnostic to prevent geom errors in large scale simulations.
Deliverables and timeline	an AI-based application detecting discrepancies between simplified CAD geometry specifications and Geant4 geometry models: prototype in FY27, productized in FY28
Personnel	M.Potekhin, S.Rahman

# Intellectual Merit Summary

This proposal addresses hard-to-tackle, advanced topics of high relevance for the high quality, efficient simulations required by multiple experiments in Nuclear and High Energy Physics, and of direct relevance to ePIC/EIC. It leverages prior experience of its participants to create specific enhancements to the Geant4 simulation toolkit, motivated by its evolving requirements.

It has the potential to benefit the ePIC/EIC effort, the BNL community and the science community at large. This work will help **advance collaboration between BNL and JLab** in the area of advanced simulations, which is important due to resident Geant4 expertise at JLab and the role of the two labs as the co-host labs for the EIC.

Importantly, this proposal comes at exactly the right time to foster close collaboration between the BNL staff and **world-class Geant4 experts who have already expressed interest in our work** (as stated in the letter from Dr. Makoto Asai – attached), thus creating a definitive **leadership position** for Brookhaven National Laboratory in this area of expertise.

# Return on Investment

- Increased efficiency of simulations (such as these of optical photons), when operating in heterogeneous computing environments involving accelerators (e.g. GPUs). This will be important for a few experiments, such as ePIC, DUNE and others.
- More precise simulations of the X-ray processes, central to the design and characterization of the IR of the EIC and future accelerators. Improved accuracy of simulations will improve the quality of the design of these crucial components, thus enhancing the science reach of the EIC.
- Robust simulation geometry validation, which will reduce the possibility of simulation errors and lost productivity.
- Increased level of Geant4 expertise at the Lab and its profile in the area of advanced simulation techniques.

# The Broader Impact on the Laboratory

For the first time in BNL history, two of its employees were invited to join the Geant4 Collaboration in 2024. In addition to the increased profile of Brookhaven National Laboratory as a knowledge center in the NP/HEP simulations, this created an opportunity to benefit from direct contact with foremost experts in this field, formulating new requirements and receiving expedited expert advice on advanced topics.

However, this also entails the responsibility to make meaningful and substantial contributions to the Geant4 toolkit, motivated by emerging requirements. Until now, our capability to do so was limited by lack of dedicated funding. This proposal creates an opportunity to meet our obligations, and in doing so cultivate in-house Geant4 expertise at BNL, at precisely the crucial time when the design of the ePIC detector is entering its most active phase. Combined with the increased engagement of the team members with the Geant4 Collaboration in the past year, this creates a uniquely opportune timing for this work to be commissioned.

# Names of Suggested BNL Reviewers

We propose the following reviewers, based on their expertise in NP/HEP simulations and computing science:

- K.Kauder (sPHENIX)
- M.Lin (Computing and Data Sciences)
- B.Viren (DUNE)
- J.Webb (STAR)

# If ECA Eligible – How this LDRD Benefits Your Application

This project will directly support one participant of the current proposal in applying for an Early Career Award (ECA):

- A.Natochii

This project will cover the period of FY27-FY28, and this timeline ensures that A.Natochii will meet the eligibility requirements, as he defended his Ph.D. thesis in 2019, and will have at least 3 years of eligibility remaining at the time of submission. Through this LDRD, A.Natochii will aim to make substantial contributions to the Geant4 simulation toolkit, positioning himself as an emerging expert in this critical area of HEP and NP.

This project will provide the necessary expertise and research framework to secure future funding through the ECA. Additionally, it will help the participant establish a long-term R&D program that contributes to the EIC project and other DOE missions in HEP and NP.

# LDRD Funding Table from BOM

<b>Resource Category</b>	<b>FY27</b>	<b>FY28</b>
<b>Salary, wage &amp; fringe</b>	140,354	145,867
<b>Travel</b>	11,000	5,200
<b>Total direct costs</b>	151,354	151,067
<b>Total organizational burden</b>	18,106	18,817
Procurement (Material Handling)	770	364
Common Institutional Support	79,770	79,753
<b>Total Laboratory Burden</b>	80,540	80,117
<b>Total Program Costs</b>	250,000	250,000