Brookhaven National Laboratory

U.S. DEPARTMENT OF ENERGY

FY27 NPP LDRD Type B Pre-Proposal

Development of advanced features for the Geant4 simulation toolkit

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Proposal title: Development of advanced features for the Geant4 simulation toolkit

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Indicate if this is a cross-directorate proposal: Yes ✔ No___

If yes, identify other directorates/organizations: EIC

Proposal Term: From: 10/01/2026 To: 09/30/2028

Proposal Title and Abstract

Title: Development of advanced features for the Geant4 simulation toolkit
Program: NP, HEP, EIC

We propose the development of new features in the essential NP/HEP simulation toolkit, covering the following areas:

- Internal scheduling logic for efficient utilization of heterogeneous computing resources
- Improvement of physics models used in Geant4
- Application of AI for efficient and robust validation of simulated geometry vs CAD

The proposal leverages the expertise of the project participants, developed over the past few years while working on the EIC components and the ePIC detector simulations. It also enhances the BNL status of having its personnel as official Geant4 collaboration members.

Combination of ongoing analyses of the RHIC data (including sPHENIX) and the active phase of the EIC detector design is likely to create further funding opportunities.

Advancements in the quality and computational efficiency of simulations of the detectors for the EIC, as well as the Interaction Regions of the EIC will create a positive impact across multiple work areas at the Lab. Importantly, it will ensure close cooperation with the core team of leading Geant4 developers and help advance expertise of the BNL personnel in this crucial R&D area.

Total planned funding per year in FY27 and FY28: $500,000

Description of the LDRD (1)

Developing a dedicated interface between GPU and CPU for Geant4 Simulations

Motivation	At present time, simulation of optical photons and other types of particles, aided by GPUs or other kind of accelerators, leaves the accelerator hardware underutilized by forcing it to work with the CPU in a strictly serial pipeline. This creates the accelerator (e.g. GPU) idle time during the CPU stages of code execution and vice versa, thus inflating the simulation time, and cost per simulated event. This leads to a substantial loss of performance and computational efficiency.
Proposed Development	A new, concurrent design of the CPU–GPU interface, to turn it from a bottleneck into a throughput engine.
Key Design Points	● Optimization of concurrency: we will leverage recent advancements (December 2025) in the core Geant4 code to exploit sub-event level parallelism in the context of GPU applications in ways not available to us before. This will offer further optimization of workload distribution on heterogeneous computing platforms, with a view to increase throughput.
Impact	● Creation of a highly performant execution engine for accelerator-enabled software will benefit a variety of simulation projects in HEP and NP, including development of the EIC components and the ePIC detector, and the potential second EIC detector. This will also enhance the outcome of the ESI project currently underway at BNL. ● Potential significant speed-up of simulations involving optical photons, which is often the case in the intensity frontier experiments.
BNL advantage	● Enhance the in-house expertise in emerging advanced simulation techniques which are now being actively developed in the HEP and NP communities, giving BNL the leadership status in this area.

Description of the LDRD (2)

Advanced X-ray Tracking and Surface Interaction Modeling in Geant4

Motivation	Synchrotron-radiation (SR) X-ray photons are one of the dominant sources of beam-induced backgrounds in the tracking systems of general-purpose spectrometers at electron/positron accelerators such as FCC-ee, EIC, and SuperKEKB. Current Geant4 photon reflection models do not comprehensively describe realistic beam-pipe surfaces, leading to systematic uncertainties and inefficient, CPU-intensive background simulations.
Proposed Development	Extend the native Geant4 X-ray tracking and reflection physics to enable fast and realistic detector background simulations: ● Early X-ray selection and filtering tailored to accelerator and interaction region environments ● Improved and optimized modeling of X-ray transport in vacuum beam pipes ● Extension of surface interaction physics beyond ideal specular reflection
Key Physics Extensions	● Diffuse X-ray reflection models to account for surface roughness ● Optional parametrized surface-response models for fast simulations
Computational Enhancements	● Integration with Geant4 internal scheduling for sub-event parallelism ● Design compatible with GPU acceleration for X-ray-dominated workfloads ● Reduced tracking of irrelevant photons through physics-driven early termination
Impact	● More accurate and realistic detector background predictions ● Significant reduction in CPU time for SR/X-ray simulations ● Improved reliability of the detector and interaction region designs ● Direct application to future electron/positron accelerator projects
BNL advantage	● Leverage in-house expertise in Geant4 development, SR background simulations across HEP and NP programs, with direct application to the detector design optimization ● Active collaboration with Geant4 core development community

Description of the LDRD (3)

AI-Assisted CAD ↔ Simulation Geometry Validation

Motivation	During large-scale detector construction such as ePIC, engineering designs (CAD) and simulation geometry specifications (such as Geant4/DD4hep) often diverge. Manual cross-checks are time-consuming, error-prone, and poorly scale with detector complexity. Undetected inconsistencies can lead to inaccurate background estimates and expensive late-stage design corrections.
Proposed AI Application	● Develop an AI-assisted workflow to automatically compare simplified (e.g. envelope level) CAD geometries with their corresponding detector models – such as Geant4/DD4hep used in ePIC. ● Focus on provided simplified CAD files to keep the problem traceable and directly relevant.
Key Capabilities	● Automated detection of geometry discrepancies (missing volumes, overlaps, misalignments, material mismatches). ● AI-driven identification and classification of inconsistencies beyond simple boolean geometry checks. ● Visualisation of detected discrepancies in the event display or dedicated geometry viewers.
Impact	● Early identification of geometry inconsistencies during detector construction and integration. ● Improved reliability of the detector background and radiation simulations. ● Reduced engineering-simulation feedback cycle time, supporting schedule and cost control.
BNL advantage	● Ensured consistency among various geometry models used in the design of the EIC, and the design of the various detector components such as in ePIC will reduce risk in the development of key elements of the EIC program. This work item will create a unique pool of expertise in applying AI techniques to experimental physics at the Lab, which will be well aligned with the priorities of the DOE..

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Summary

Geant4 is the key simulation toolkit used in High Energy and Nuclear Physics, as well as in a wide variety of other research areas. Efficient and cost-effective utilization of this toolkit in the modern era of large and complex detectors presents a number of challenges. This proposal includes a few distinct work areas aiming to address these challenges:

- Introduction of optimal scheduling logic for efficient utilization of heterogeneous computing resources, maximizing the concurrent use of CPU and accelerator hardware.
- Advanced X-ray Tracking and Surface Interaction Modeling, aiming to improve the models currently use in Geant4, both from the accuracy and performance standpoints.
- Application of AI for automation of complex and error-prone tasks performed in the course of complex detector simulations.

We believe that successful execution of this proposal will make a large positive impact on the research conducted at the Lab, by optimal use of the latest Geant4 features in research conducted at BNL, and as a venue of influencing future development of that crucial toolkit by participating in the Geant4 Collaboration.