

Fermi National Accelerator Laboratory

LDRD Project Data Sheet – FY20

Project ID: FNAL-LDRD-2020-050

Project title: Numerical Integration on GPUs

Principal investigator: Marc Paterno

Project description: (short description and explanation of cutting edge, high-risk, high-potential science or engineering)

This project will develop a scalable software library for large-scale high-dimensional numerical integration on emerging high-performance architectures with Graphical Processor Units (GPUs). The objective of the library is to hide the complexity of programming GPUs and make the library available to diverse applications arising in Physics. This library will enable accurate calculation of integrals of dimensionality not feasible with currently available software. Our choice to develop this library for GPU-based systems is driven by the fact that the three upcoming future DOE Exa-scale systems will all be GPU-based: Frontier (at ORNL will use AMD GPU), Aurora (at ANL will use Intel GPU), and El Capitan (at LLNL will use GPUs, vendor not finalized).

Tie to Mission: (explain the project's relevance or anticipated benefits to Fermilab's and DOE's missions)

The task of high-dimensional numerical integration is often encountered in physics, e.g., in HEP event generators like Sherpa and MADGRAPH, in Bayesian parameter estimation, and in models of physical systems. Dramatic improvement in integration algorithms, combined with vastly increased computational resources available on modern supercomputers, can bring into reach the ability to model the complicated relationships between cosmological and astrophysical parameters. This will improve both the accuracy and precision of cosmological measurements. Improvements to the predictive capabilities of event generators will help us extract the full potential of investments in the LHC.

Previous year's accomplishments: (as applicable)

Identified the DES experiment to apply techniques. Began Design of efficient algorithms.

Work proposed for current fiscal year and anticipated / desired results:

Explore use of portable programming libraries/languages for algorithm implementation. Explore how to leverage multiple GPUs.

Project funding profile: (costs, budgets, projected budgets, and total)

| Prior year(s) costs | FY20 ½ | FY21 | FY22 | FY23 ½ | Total |
|---------------------|--------|---------|--------|--------|---------|
| N/A | 43,675 | 114,233 | 52,092 | | 210,000 |

Project Start Data: 3/1/2020

Total Approved Project funds: \$210,000