Optical sims using GPUs



Nersc Users Group Lightning Talk

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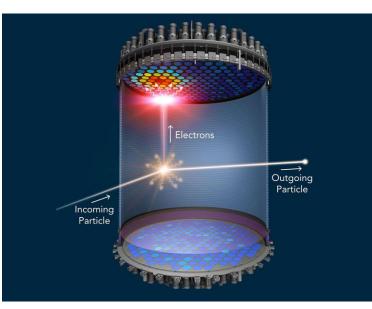
Oisín Creaner¹, Maria Elena Monazi², Lisa Gerhardt¹, Quentin Riffard³, Sam Eriksen⁴ ¹LBNL/NERSC, ²Stanford University/LZ, ³LBNL/LZ, ⁴University of Bristol/LZ 17th August 2020 LZ

- •LUX-ZEPPLIN (Large Underground Xenon ZonEd Proportional scintillation in Llquid Noble gases)
- •Next-generation Dark Matter detector
- Particle interactions with the Xenon detection medium
- •Compare with simulated interactions.
- •Photon propagation: time- and resource-intense



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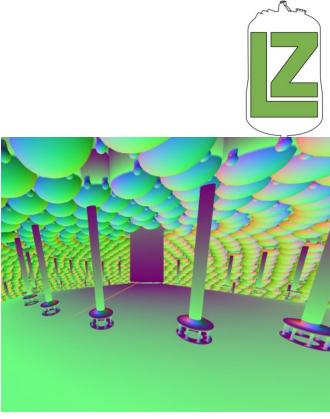




Motivation to GPUs

•Replace existing CPU module with GPU solution

- Photon propagation is simulation bottleneck
- Faster simulations
- More frequent simulations
- Better use of available hardware
- •Opticks: A GPU Accelerated Optical Photon Simulation using NVIDIA OptiX



Blythe, S (2019) Renders of the chimney region of JUNO detector as an Opticks Geometry

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LZ at NERSC

- •LZ is major NERSC user
- Simulations: CPU based
 Data storage
 Data analysis:
- •Mock Data Challenge Science Run 1 starting soon!
- Existing Optics implementation Local/Cloud Move to CoriGPU Prepare for Perlmutter

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NERSC, 2019

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Containerisation: Docker and Shifter

•Shifter:

- Security requirement to run on CoriGPU (and Perlmutter)
- o Build a docker image, export to Shifter to run
- READ ONLY and NO ROOT ACCESS

•Docker:

- $\circ~$ Write Dockerfile with all commands required to build
- Create image with all dependencies and specific versions
- Should be very portable: solution should continue to work when upgraded

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Challenges in creating an image

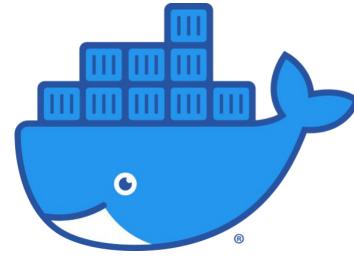
- Many undocumented assumptions
- •Hard-coded or semi-hard-coded (e.g. \$HOME) paths
- •Hardware awareness of compiled libraries
- Security restrictions on writing
- •Unexpected write commands buried deep in layers
- •NVidia Runtime mismatch with drivers
- •Specific version and/or commit dependencies







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Solutions

- Containerisation & Portability
 - Versions locked in when image created
- Fork development from stable point
- Identify assumptions and hard-coding and make soft links
- Mount data in writable partitions (e.g. \$SCRATCH)
- Hardware-aware compilation has to happen on the correct host















Optical sims using GPUs

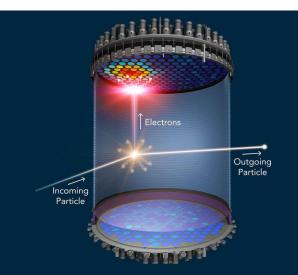
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Image References

Blythe, S, 2019 Opticks : GPU Optical Photon Simulation for Particle Physics using NVIDIA® OptiX[™]. EPJ Web of Conferences 214, 02027

NERSC 2019, Cori Supercomputer