Summary of Research Work in PocarLab

Advisor: *Professor Andrea Pocar*

Duration: *May, 2024 - December, 2024*

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Executive Summary

This presentation highlights my contributions and growth during my time in the PocarLab, focusing on GPU-based optical simulations and detector design for the nEXO collaboration.

Key Highlights:

- **Chroma Simulation Comparisons:** Systematic analysis of SolidWorks vs. Fusion360 geometries, investigating photon transport efficiency and tessellation effects.
- **Detector Optimization Studies:** Exploration of silicon reflector heights and alternative detector cell configurations to maximize photon collection and experimental flexibility.
- **Simulation Troubleshooting:** Diagnosed and mitigated PyCUDA errors, improving stability and workflow efficiency for large-scale simulations.
- **Lab Contributions & Collaboration:** Supported experimental setups, strengthened simulation-hardware integration, and collaborated on workflow improvements.
- **APS DNP 2024 Conference:** Presented research nationally, demonstrating technical expertise and communication skills.
- **Skills & Growth:** Developed technical, scientific, and soft skills that have enhanced my research abilities and prepared me for my next astrophysics project.

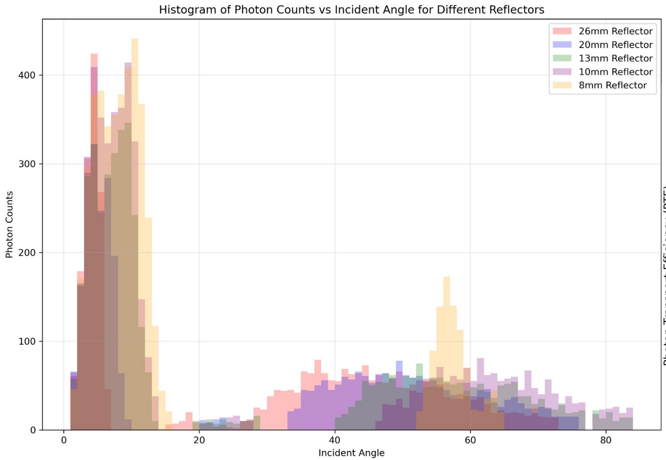
Exploring Chroma Simulation Discrepancies: A Comparative Analysis of SolidWorks and Fusion360 Geometries

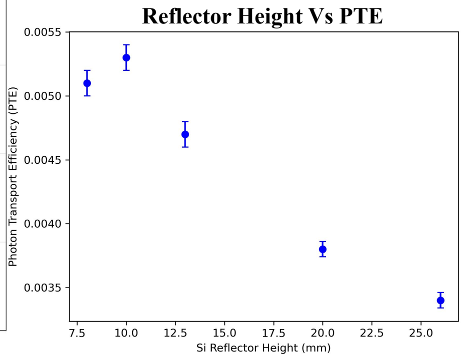
- **Objective**
    - Investigated discrepancies in photon transport simulations using geometries created in SolidWorks vs. Fusion360.
    - Aimed to determine if Fusion360 could replace SolidWorks in the lab — a cost-efficient and scalable alternative.
- **My Role**
    - Designed and exported identical detector geometries in both CAD tools with controlled material/surface properties.
    - Set up, executed, and analyzed Chroma simulations for both models using 1,000,000 photon events per run.
    - Developed scripts and workflows to standardize geometry imports, run parameterized simulations, and extract PTE metrics.
- **Key Results**
    - Found minor (<1%) PTE difference between SolidWorks (0.01336) and Fusion360 (0.01324) geometries: statistically insignificant ($p = 0.1112$).
    - Discrepancies traced to STL resolution and tessellation quality, not fundamental geometry or material differences.
    - Discovered that higher mesh resolution improves reflected photon capture (PTE goes up with finer tessellation).
- **Deeper Analysis**
    - Conducted systematic PTE vs. resolution tests:
        - SolidWorks: “Extra Fine” vs. “Coarse” → 5.3% PTE difference.
        - Fusion360: Low → Medium → High → consistent PTE increase.
    - Identified primary parameters affecting tessellation:
        - SolidWorks: Deviation Tolerance
        - Fusion360: Surface Deviation
- **Outcome & Impact**
    - Concluded that Fusion360 (Medium) and SolidWorks (Custom Extra Fine) produce interchangeable results if settings are standardized.
    - Provided the lab with recommendations for STL export protocols, improving reproducibility and accessibility.
    - Findings allowed multiple workstations to run geometry creation and Chroma simulations without reliance on limited SolidWorks licenses.

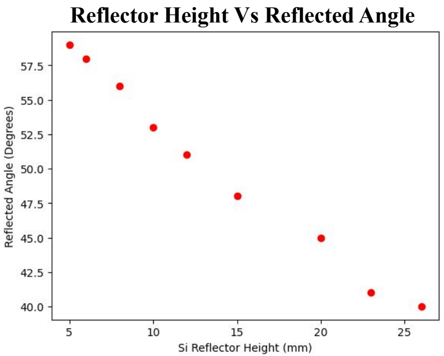
Link to the Internal Lab Memo: [20240809 Chroma_SolidWorks Vs_Fusion_Comparison_Test.pdf]

Silicon Reflector Height Analysis

- **Objective**
  - Investigated how varying silicon reflector heights influence photon transport behavior in the simulation.
  - Aimed to determine the optimal reflector height for maximizing photon collection efficiency and reflected light uniformity in the detector setup.
- **Approach**
  - Created five geometry variants with reflector heights: 8 mm, 10 mm, 13 mm, 20 mm, and 26 mm.
  - Simulated photon transport in each geometry using identical Chroma parameters.
  - Analyzed photon transport efficiency (PTE), incident-angle distributions, and reflected-angle trends.
- **Key Results**
  - Photon Transport Efficiency (PTE) decreased steadily with increasing reflector height (see blue plot).
    - 8 mm → highest PTE (~0.0051), 26 mm → lowest (~0.0034).
  - Reflected Angle showed a clear inverse relationship with height (see red plot):
    - Taller reflectors → smaller reflection angles (more vertical incidence).
  - Incident-Angle Histograms show two clear peaks:
    - ~0–15° (direct hits) and ~55–60° (reflected hits).
    - The reflected-hit peak weakens as height increases, indicating reduced reflective contribution at larger heights.







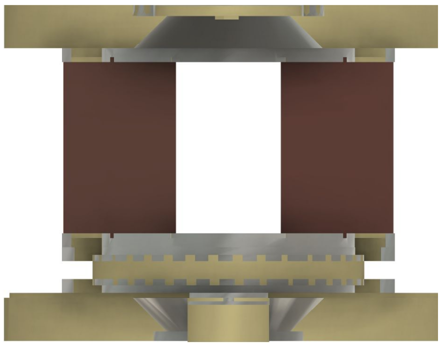
Total Photon Counts for Angles > 30

#	Reflector Height	Total Photon Counts
1	26mm Reflector	1851
2	20mm Reflector	1849
3	13mm Reflector	1694
4	10mm Reflector	1650
5	8mm Reflector	945

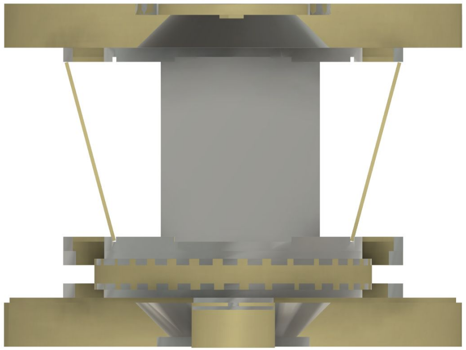
Photon counts plateau beyond ~20 mm, showing diminishing returns in photon collection above this height.

Alternate Cell Configuration Analysis

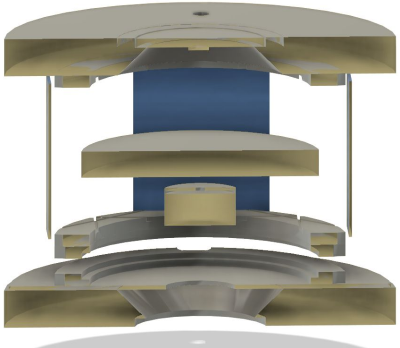
- **Objective**
  - Proposed and evaluated alternative detector cell configurations to enhance information extraction and experimental flexibility.
  - Explored one additional measurement method (optical measurement of refractive index using ellipsometry) to complement the new geometries.
  - Aimed to assess feasibility, buildability, and potential performance gains before running full Chroma simulations.
- **Key Questions**
  - Are these configurations mechanically and experimentally feasible to build in the lab?
  - Some options require additional liquefaction cycles — how practical are they to perform regularly?
  - Which configurations are most promising for next-phase simulation and testing?
- **My Role**
  - Collaborated with Luc Barrett and Loick Marion on concept development.
  - Designed detailed 3D geometries in SolidWorks for all proposed configurations.
  - Ensured mechanical accuracy and compatibility with existing Chroma simulation frameworks.
- **Impact**
  - Opened pathways for innovative detector configurations that could provide richer diagnostic data.
  - Improved our understanding of engineering constraints in experimental cell design.
  - Strengthened collaboration across simulation and hardware teams within the lab.



Current Setup: 4-outer



Tilted Reflectors: 4-outer



Different Source-SiPM Distance

PyCUDA Error Investigation

- **Objective**
  - Investigate the recurring PyCUDA “illegal memory access” error encountered during Chroma simulations.
  - Identify possible underlying causes and propose strategies to mitigate the issue.
- **Background**
  - PyCUDA handles GPU-based photon propagation in Chroma simulations.
  - Errors occurred inconsistently across geometries, halting simulation runs and reducing throughput.
- **Hypothesis — Back-Face Culling as a Potential Cause**
  - Back-face culling: a graphics optimization technique that removes polygons not visible to the viewer.
  - Possible issue:
    - The algorithm may incorrectly cull visible faces due to improper surface normal orientations,
    - leading to GPU memory access violations during photon tracing.
  - Suggests a geometry-dependent rendering conflict between Chroma’s ray-tracing engine and CAD exports.
- **Observed Behavior**
  - Reducing the total number of photons eliminates the PyCUDA error.
  - Error disappears consistently when photon count decreases from 1,000,000 → 999,995–999,999, varying by geometry.
  - Indicates a possible memory allocation threshold or buffer overflow condition related to photon batching.
- **Approach**
  - Conducted controlled tests varying photon counts, geometry complexity, and GPU memory usage.
  - Exploreed modifications to back-face culling parameters or mesh normal consistency checks.
- **Impact**
  - Enhances simulation stability and reliability for all GPU-based Chroma analyses.
  - Prevents lost runtime and GPU crashes during long simulations.
  - Contributes toward a more robust and error-tolerant workflow for large-scale optical modeling.

General Lab Contributions

- **Core Responsibilities**
  - Designed 3D detector geometries in SolidWorks for integration with the Chroma optical simulation framework.
  - Executed and analyzed Chroma simulations to generate data for ongoing detector performance studies.
- **Experimental Support**
  - Assisted in assembling the SiPM enclosure and setting up the experimental cell alongside Ed.
  - Helped ensure mechanical alignment, component sealing, and integration with optical components.
- **Collaborative Development**
  - Worked extensively with Luc Barrett and Loick Marion to:
  - Improve Chroma's simulation efficiency and reliability.
  - Test and benchmark new code implementations.
  - Provide detailed technical feedback on bugs, inconsistencies, and optimization opportunities.
- **Outcome**
  - Contributed directly to the development of the "New Chroma" simulation pipeline, improving speed, stability, and usability for the lab's ongoing projects.
  - Strengthened collaboration between hardware and simulation teams, bridging design and computational workflows.

APS DNP CEU, Boston, Oct 2024 - *Fully funded by APS, NSF, and UMass Amherst Physics Department*

Effect of Surface Resolution on Ray-Tracing Optical Simulations

- **Overview**
    - Selected to present research at the American Physical Society – Division of Nuclear Physics (APS DNP) Conference.
    - One of a limited number of undergraduates nationwide chosen for the Conference Experience for Undergraduates (CEU) program.
    - Received full funding from the APS, NSF, and UMass Amherst.
- **Research Presented**
    - Project Title: Exploring Chroma Simulation Discrepancies: A Comparative Analysis of SolidWorks and Fusion360 Geometries
    - Part of the nEXO Collaboration, which aims to detect neutrinoless double beta decay in liquid xenon (LXe).
    - Used Chroma, a GPU-based ray-tracing software, to study photon transport efficiency (PTE) in LXe detector geometries.
    - Investigated how CAD model tessellation and resolution impact photon absorption on Silicon Photomultipliers (SiPMs).
- **My Contributions**
    - Designed and exported precise 3D detector geometries in SolidWorks and Fusion360.
    - Conducted systematic simulations varying tessellation resolution while controlling all physical parameters.
    - Performed comparative statistical analysis on round vs. flat reflector geometries.
    - Demonstrated that finer tessellation significantly improves photon collection efficiency, especially in curved geometries.
    - Provided recommendations to the nEXO collaboration for standardizing CAD-to-Chroma workflows for improved accuracy.
- **Key Impact**
    - Helped refine simulation-to-experiment consistency in detector optical modeling.
    - Strengthened the lab's understanding of geometry resolution effects in optical simulations.
    - Represented UMass Amherst at a national-level nuclear physics conference.

Link to the Poster: APS DNP CEU Oct 2024 Poster, APS DNP CEU Oct 2024 Abstract, APS DNP CEU Oct 2024 Contribution Statement

Skills and Tools Developed

- **Technical Skills**
  - **Programming & Computation:** Python, C++ for simulation scripting, analysis, and automation.
  - **High-Performance Computing:** GPU parallelization using PyCUDA to accelerate Chroma ray-tracing simulations.
  - **CAD & Geometry Design:** SolidWorks and Fusion360 for precise detector geometries and STL export optimization.
- **Scientific Skills**
  - **Data Analysis & Validation:** Quantitative assessment of photon transport efficiency, uncertainty quantification, and comparative studies.
  - **Simulation Validation:** Cross-checking CAD models, mesh resolutions, and ray-tracing outputs for reproducibility.
  - **Communication & Dissemination:** Writing technical reports, research papers, and conference posters; presenting at APS DNP 2024.
- **Soft Skills**
  - **Independent Research:** Self-directed problem-solving, workflow development, and simulation optimization.
  - **Collaboration & Teamwork:** Coordinated with lab members across simulation and experimental teams.
  - **Scientific Communication:** Clearly conveying complex technical findings to peers, supervisors, and national conference audiences.

Summary

- **Key Contributions**
    - Conducted systematic Chroma simulations comparing SolidWorks and Fusion360 geometries, identifying resolution-dependent PTE effects.
    - Investigated silicon reflector heights and alternative detector configurations, providing insights for optimal photon collection.
    - Diagnosed and mitigated PyCUDA errors, improving simulation stability and workflow efficiency.
    - Represented UMass Amherst at APS DNP 2024, presenting research on GPU-based optical simulations and CAD optimization.

I am deeply grateful to Professor Pocar for welcoming me into the PocarLab when I couldn't secure another research opportunity that summer. My experience in the lab—tackling simulations, diagnosing errors, and collaborating closely with the team—not only strengthened my attention to detail and made me a more rigorous scientist, but also paved the way for my transition to my current theoretical astrophysics research group, which I had been aiming to join since starting at UMass. Your mentorship has been invaluable in shaping both my technical skills and scientific mindset. Thank you.

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