Monte Carlo Simulation and Differentiable Simulator in Particle Physics

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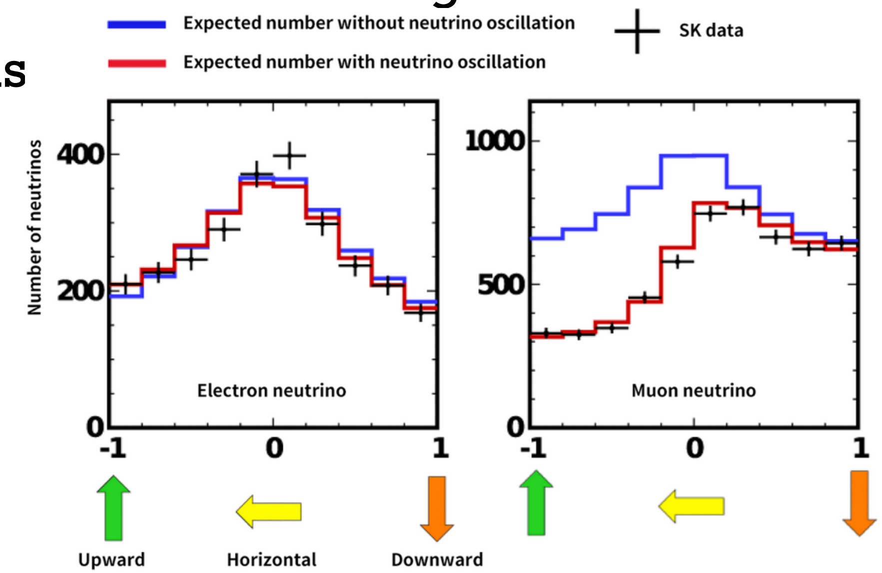
Why do we need simulation?

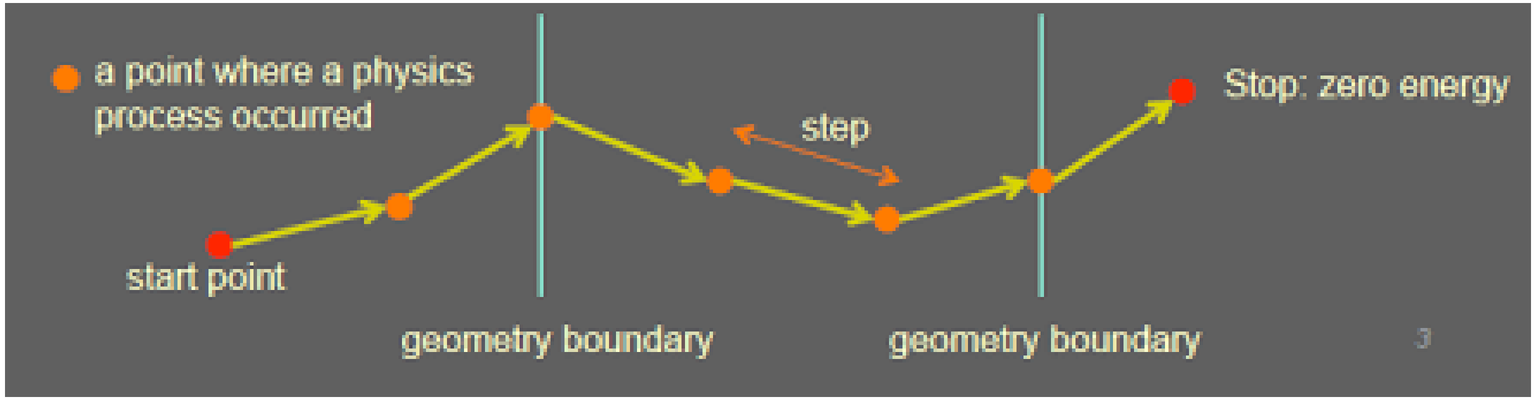
- Particle interactions are stochastic processes, analytic solutions are impossible
- Generate detector response with tunable parameters ↔ calibration
- Signal selection and background estimation
- Resolution, efficiency and acceptance of signal events
- Systematic uncertainties from inaccurate physics/detector modelling
- Produce training data for machine learning models

- Simulation vs. Real Data → Physics measurements



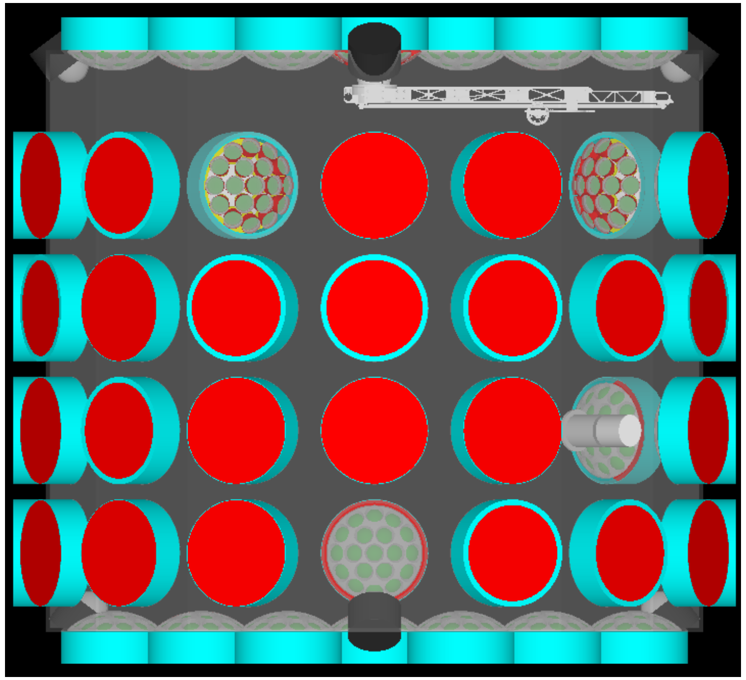
WCSim: Water Cherenkov detector Simulation

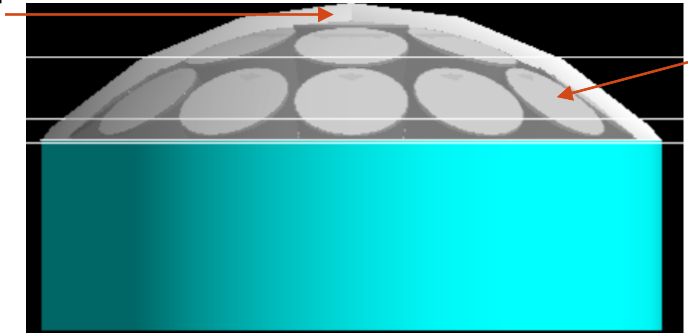
- Official simulation software in WCTE (CERN) and Hyper-Kamiokande (Japan)
- Geant4-based Monte-Carlo (MC) simulation software:
  full particle tracking from production to "dead"
- Basic ingredients
  - Geometry
  - Physics processes
  - Photomultiplier tube (PMT) electronic responses

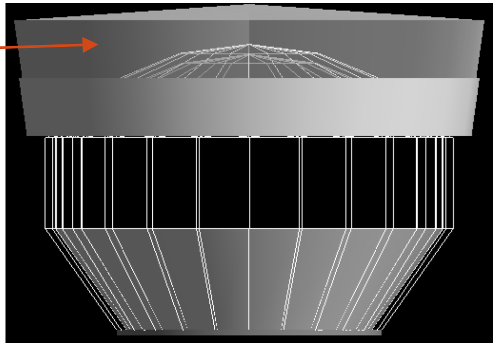


Geometry and material definition

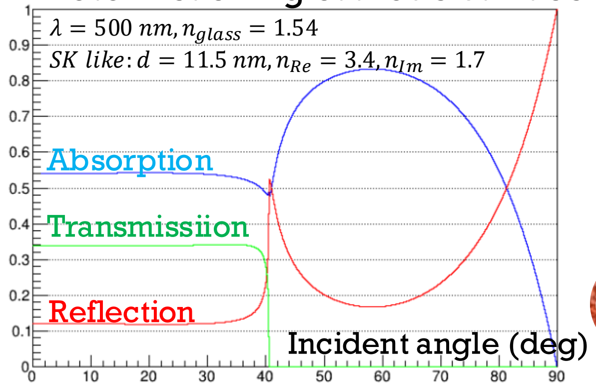
- Pure water as target volume
  - Optinal Gadolinium (Gd) doping
  - Light absorption and scattering length from Super-Kamiokande (SK)
- Blacksheet to enclose detector
  - 10% reflectivity (Lambertian/diffuse)
- Central deployment system, beam pipe, camera housing
  - Reflective surfaces
- mPMT housing + gel + PMT glass cathode
  - Refractive indices and cathod thickness decides angular response







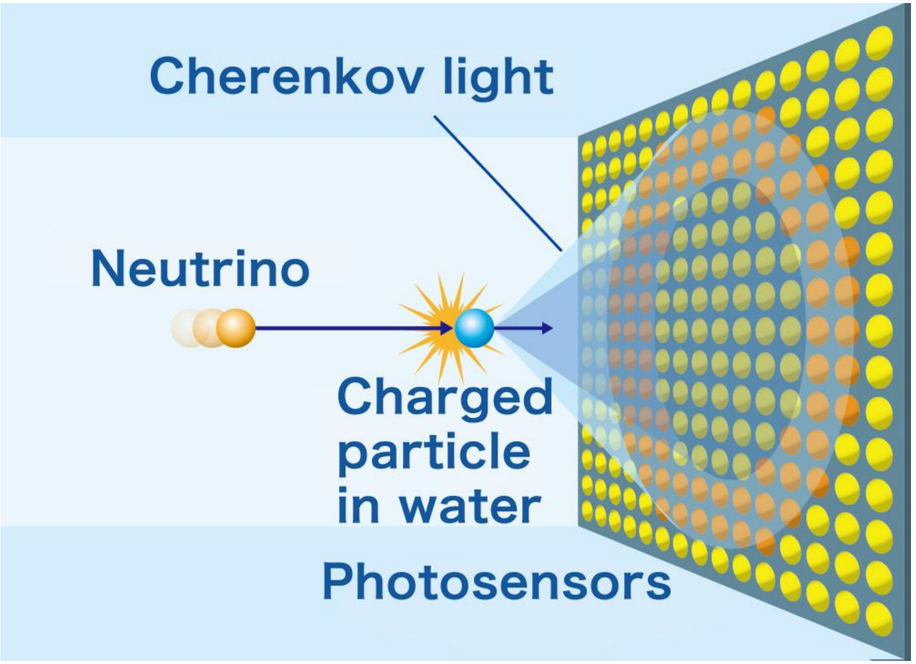
Photon reaching cathode surface

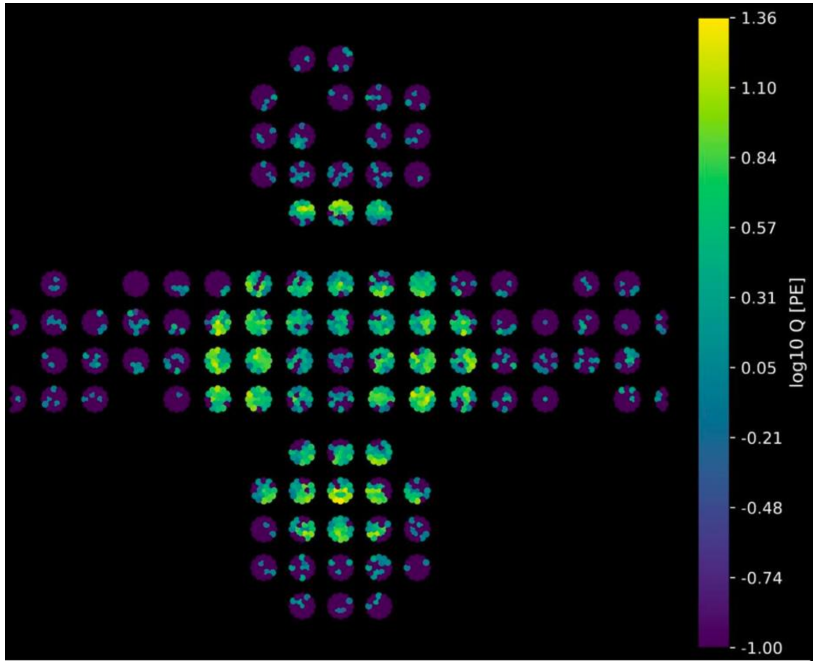


Physics processes

- GEANT4 default physics list FTFP_BERT(_HP)
  - Recommendation for collider physics and cosmic ray calibrations up to few tens of GeV
  - HP: high precision neutron models below 20 MeV
- Gd de-excitation gamma model
  - HP with photon evaporation model to enforce energy conservation, at the cost of distorting gamma energy spectrum
- Pion interaction model
  - Bertini intranuclear cascade model below 3GeV
  - cf. SK/T2K interfaces with NEUT cross sections used in FSI/SI
- **Optical photon propagation**

Water Cherenkov Detector principles





"T2K 2021 syst.": Phys. Rev. D 103, 112008

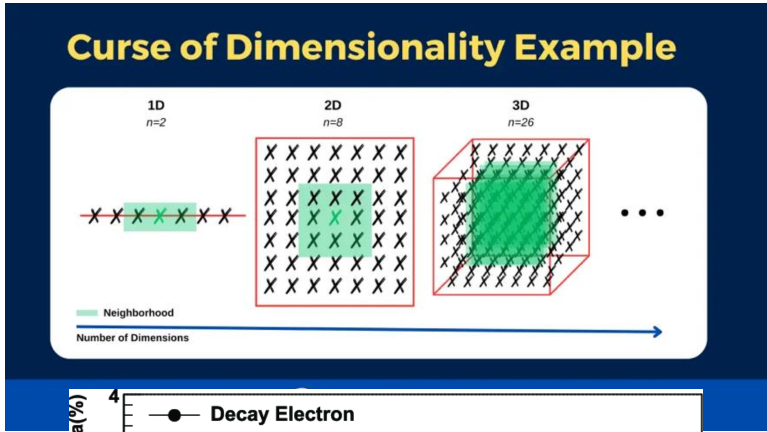
Error Source	% Error for CPV search
$\varphi + \sigma$ (ND constrained)	2.7
$\varphi + \sigma$ (ND unconstrained)	1.2
Nucleon removal energy	3.6
π re-interactions	1.6
$\sigma(\nu_e)$, $\sigma(\bar{\nu}_e)$	3.0
NC γ + other	1.5
SK far detector	1.5
Total	**6.0**

ND Fit

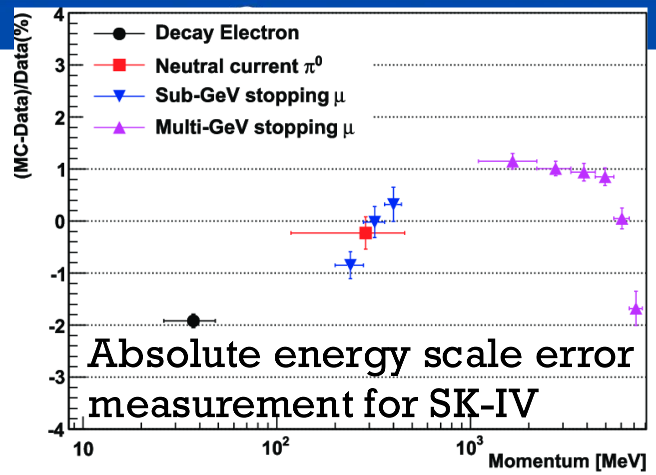
Goal for HK: 3%

- Traditionally use MC simulations tuned with calibration data to generate observables with which we use to analyze real physics data → Hard but necessary to reduce detector uncertainties to <1%

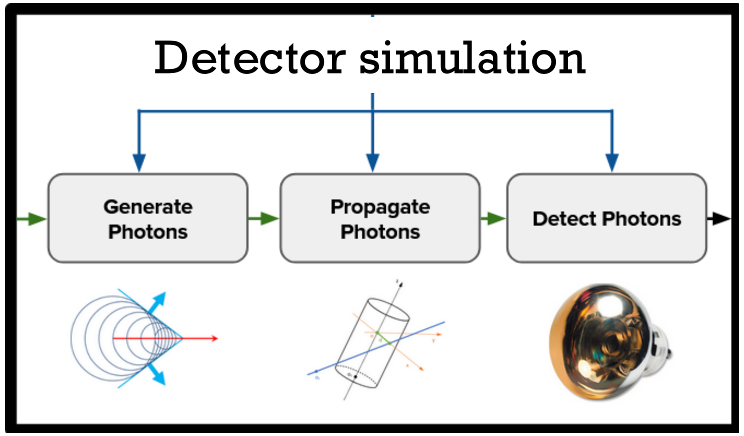
Detector Physics Modeling: Challenges

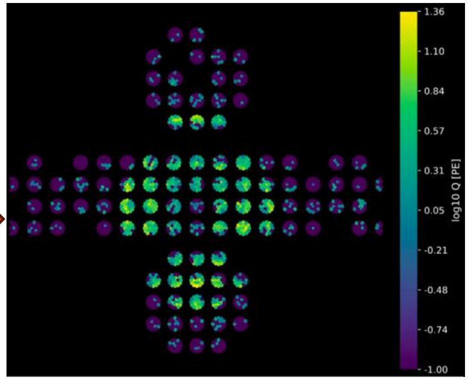


- **Quality** due to limitation in the traditional calibration
  - "one-by-one" (sequential) parameter calibration assumes weak/no correlations
  - Non-optimizable routines (e.g. look-up tables)
  - Not directly minimizing the "data-simulation discrepancy" metrics
- **Speed** for modeling a large and complex detectors without loss of quality
  - Seconds to minutes per event prevents high statistics $O(10^9)$ simulations
  - Faster = can unlock new analysis techniques (e.g. simulation-based inference)
- **Resources** for software development and maintenance
  - Same detector physics, separate software (simulation vs. calibration/reconstruction)



Track input





Detector output

Reconstruction → Reconstructed track

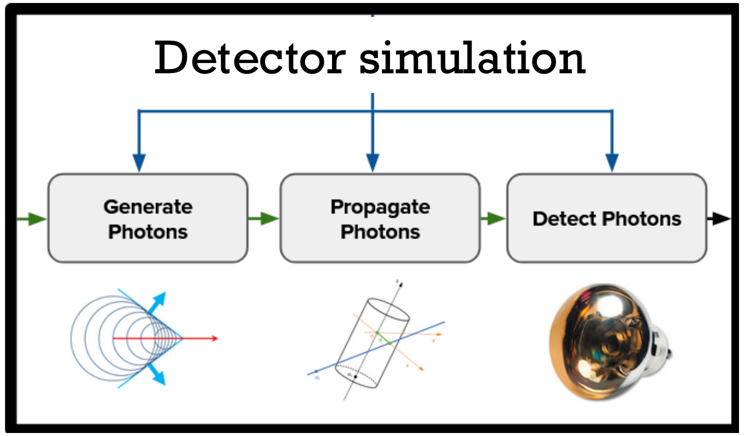
Detector physics model parameters

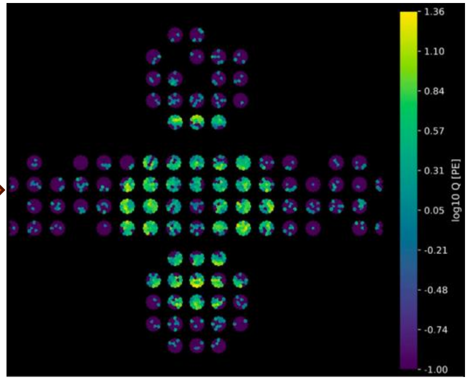
Calibration

Proposal: Differentiable Detector Simulator (DDSim)

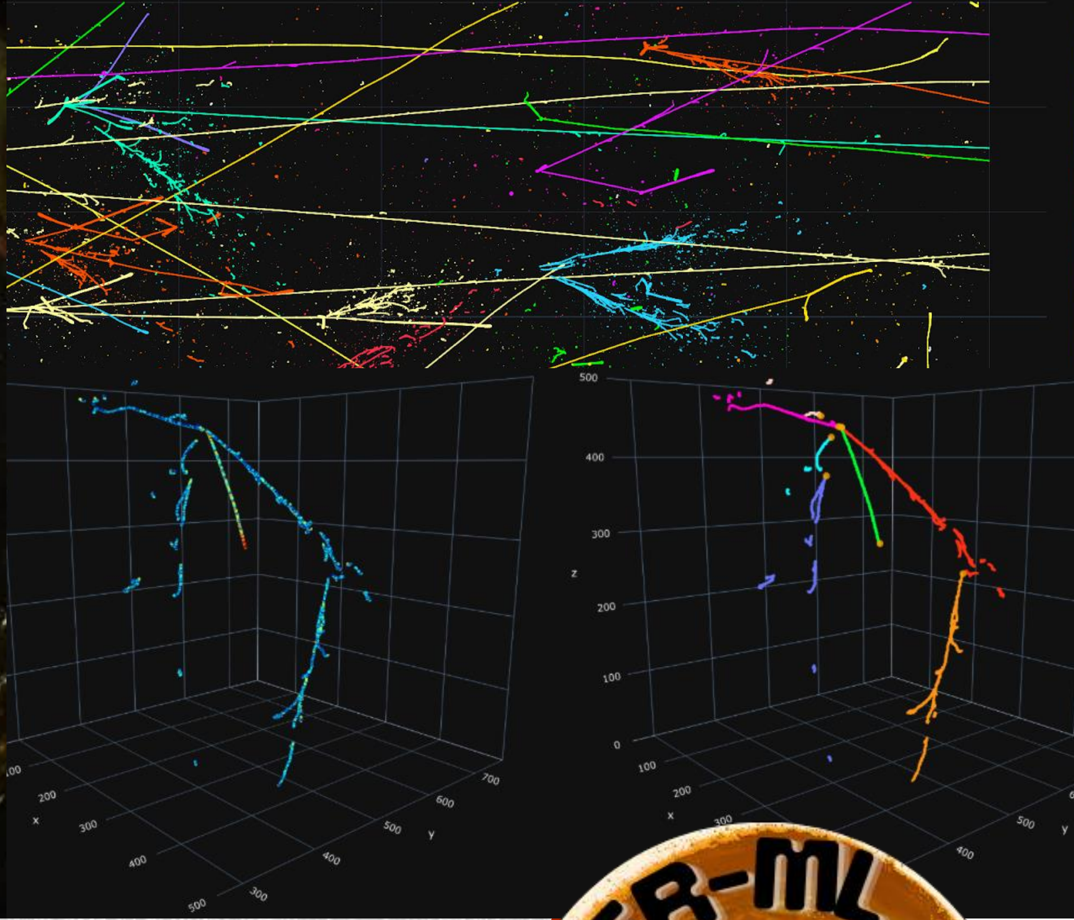
- **Automation of physics model tuning (via backpropagation)**
  - **"End-to-end"**: gradient-based optimization using calibration and physics datasets
  - **Interpretable**: analytical physics models for well-understood physics
  - **Flexible**: neural representations to incorporate complex features in real data
  - **Fast**: utilization of modern computing accelerators (e.g. GPUs)
- Proof of concept: **Differentiable Optical Detector Simulation**
  - OpticSiren, LUCiD

Track input





Detector output



CIDeR-ML Collaboration

KAVLI IPMU

SCHOOL OF SCIENCE THE UNIVERSITY OF TOKYO

東京理科大学 TOKYO UNIVERSITY OF SCIENCE

Institute of SCIENCE TOKYO

SLAC

UNIVERSITY OF MINNESOTA

Stanford University

Tufts UNIVERSITY

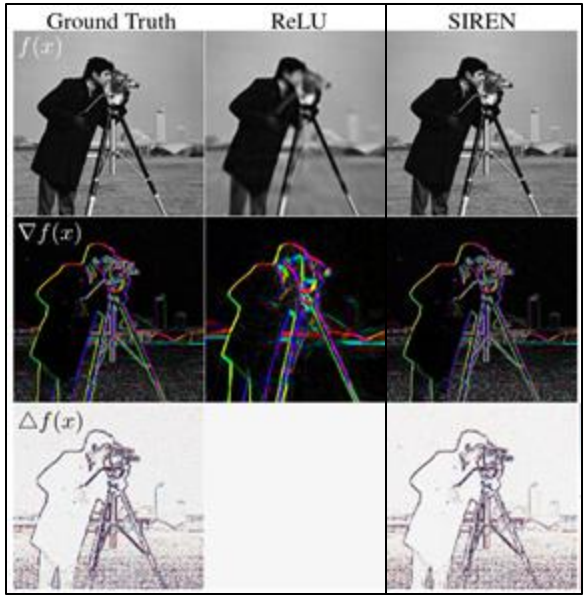
CIDER-ML

OpticSiren

- **Differentiable surrogate model for Optical processes**
- ~ **Look-up Table**: a database of per-PMT photon "visibility" for binned positions/directions
  - Scales poorly for a large detector
  - Created with simulation. Difficult to tune with data
- **Siren**: fully connected deep neural network with sinusoidal activations
  - Implicitly defined, continuous, differentiable signal representations
  - "smooth" = model the underlying physics gradient
  - Optimizable directly on real calibration dataset!

Siren

Sinusoidal Representation Network

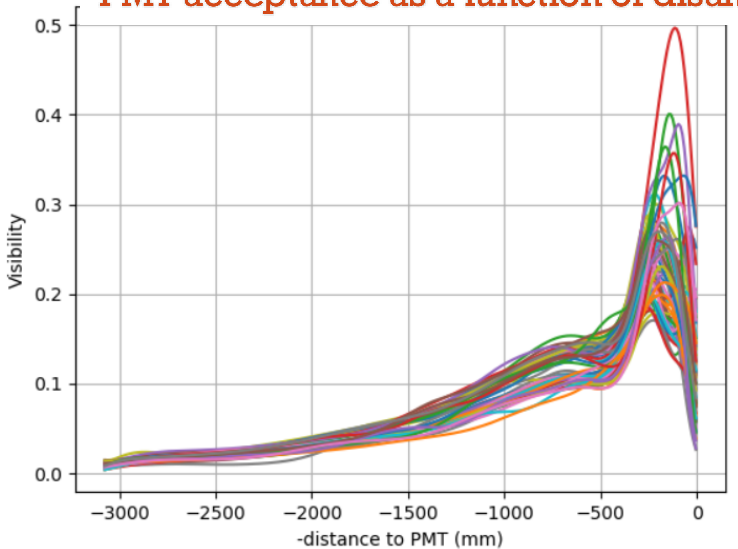


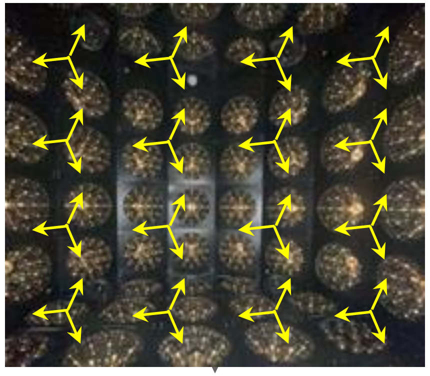
Can better represent underlying distributions and their derivative compared to other networks

Training and validation

- Demonstration in WCTE (cylinder of length ~ 3 m)
- Simulate PMT response (~2000) with WCSim for O(1M) photon starting position×direction → Look-up table as training data
  - Spatial/angular resolution matched with PMT spacing
- Direct check of physical behavior

PMT acceptance as a function of disanrce





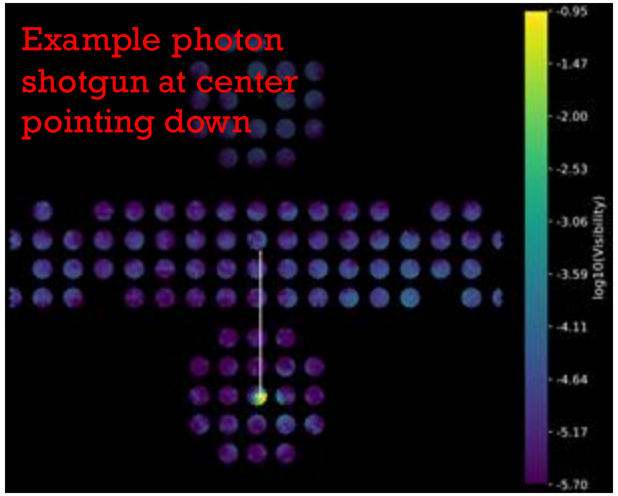
Conventional photon libraries are discrete and sampled

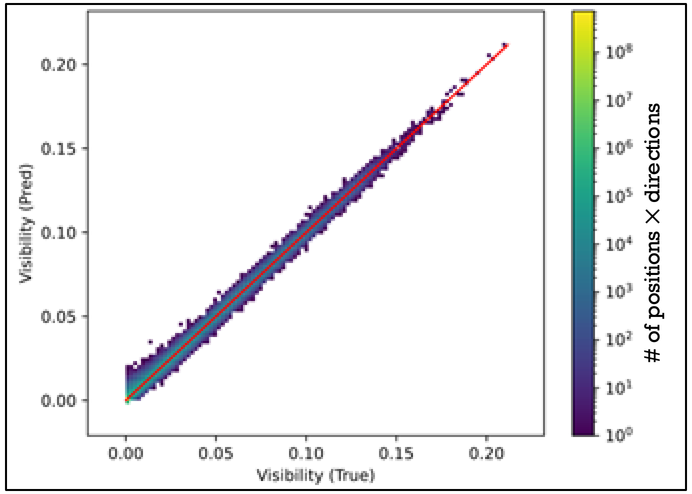
$vis(\vec{x}, \vec{d})$

SIREN

Photon Propagation

Provides continuous and differentiable photon library





visibility: probability of observing 1 photon from some position in detector

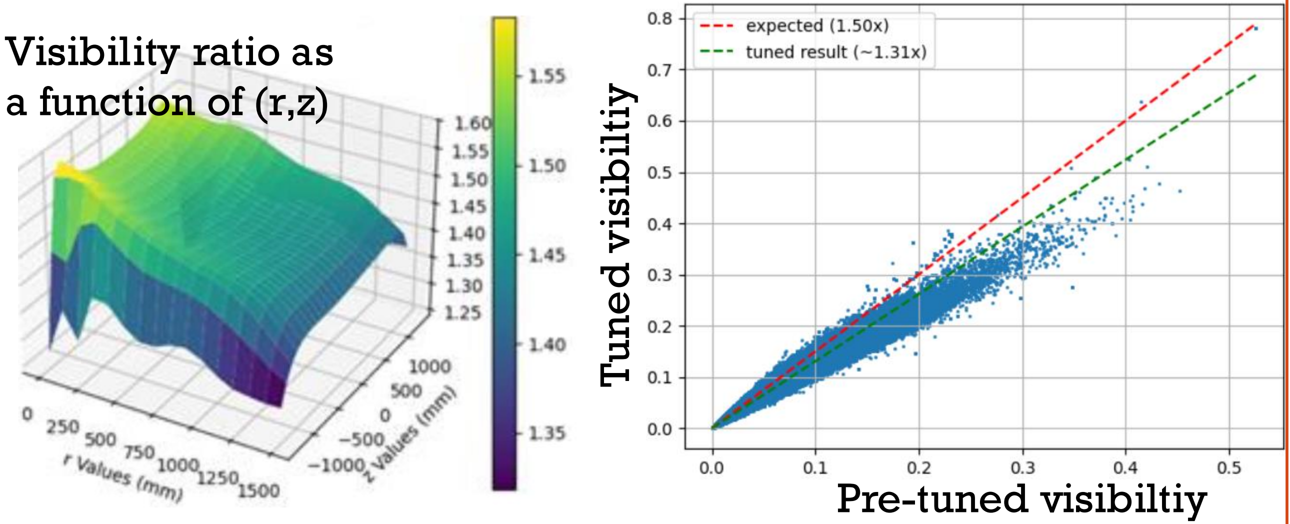
Calibration

- Fine-tuning with (fake) calibration data
  - Fixed isotropic light sources: “overfit” around the given positions
  - On going work on cosmics → span whole detector

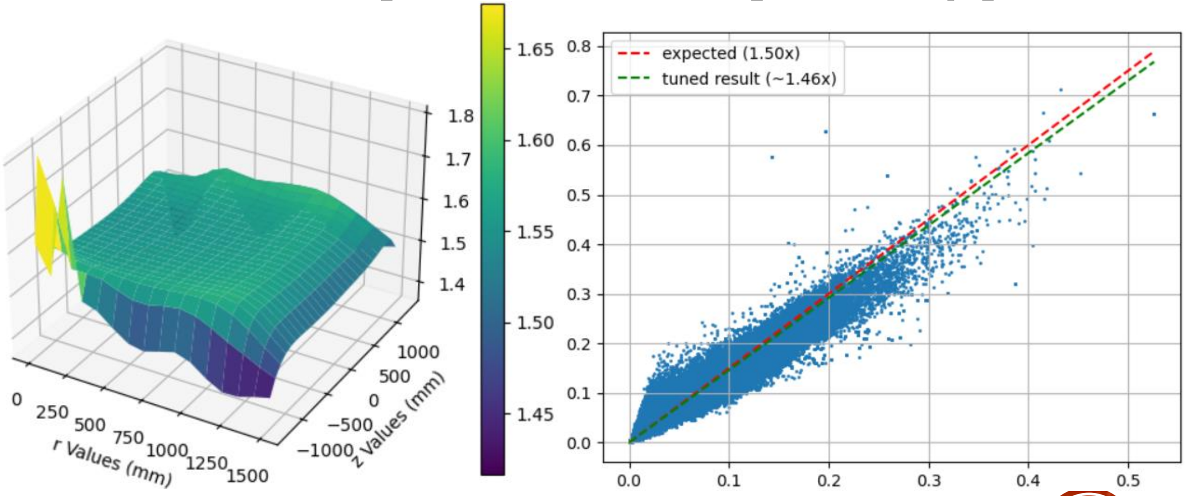
Fake calibration data with charge × 1.5

Case 1: 3 isotropic sources at (0,0,0), (0,0,-1m),(0,0,1m)

Visibility ratio as a function of (r,z)

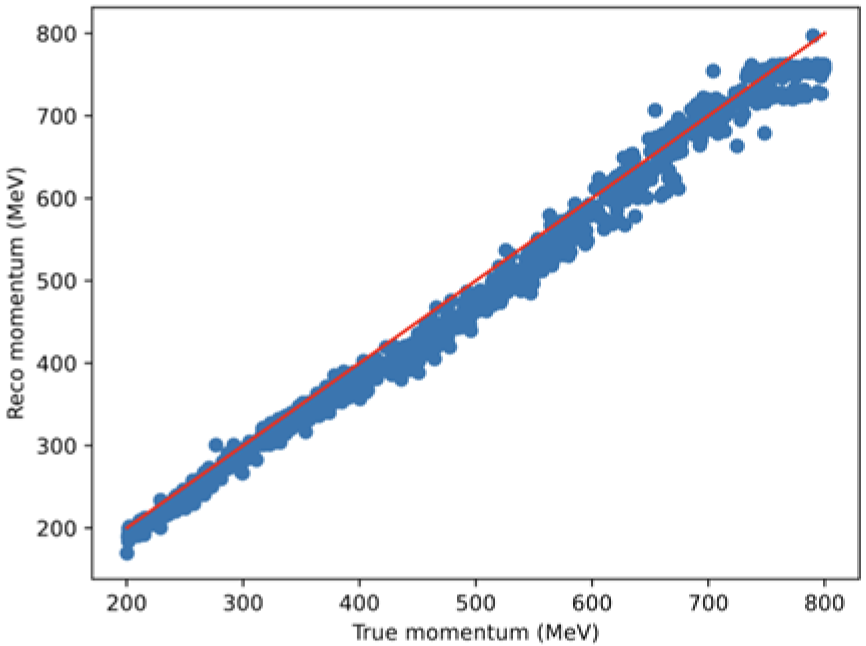


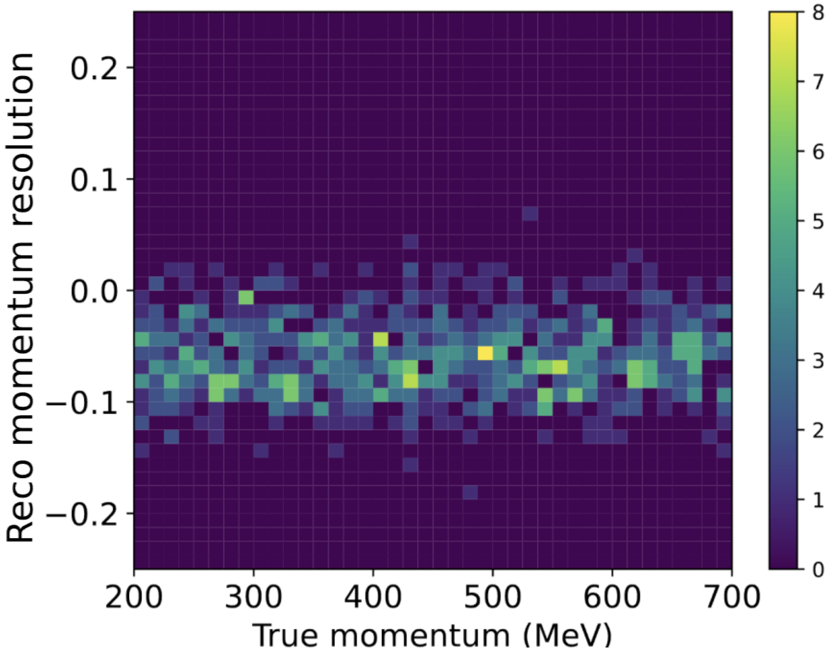
Case 2: 126 isotropic sources at 14 z-pos ⊗ 9 xy-pos



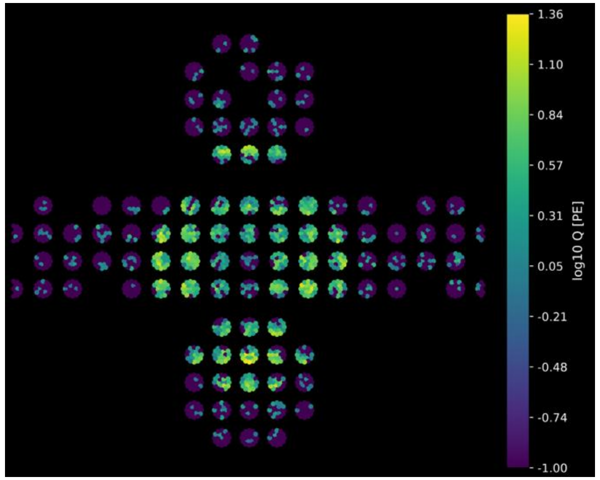
Reconstruction

- Connect the **OpticSiren** with another differentiable model of Cherenkov photon production (Cherenkov Siren)
  → optimization of track parameters
- Muon momentum reconstruction with **OpticSiren**, on WCTE MC data

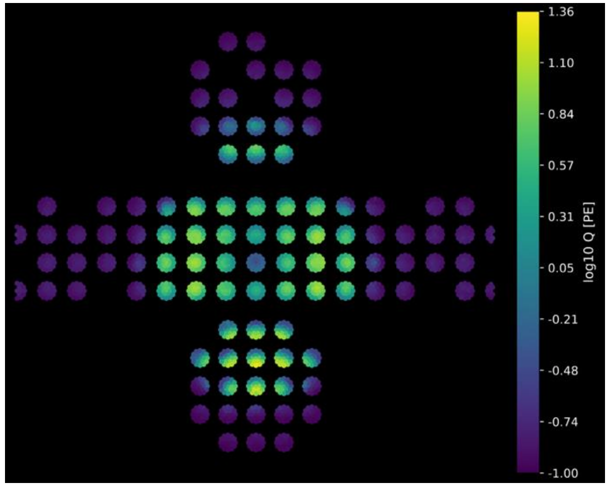




MC



Muon of 500 MeV/c



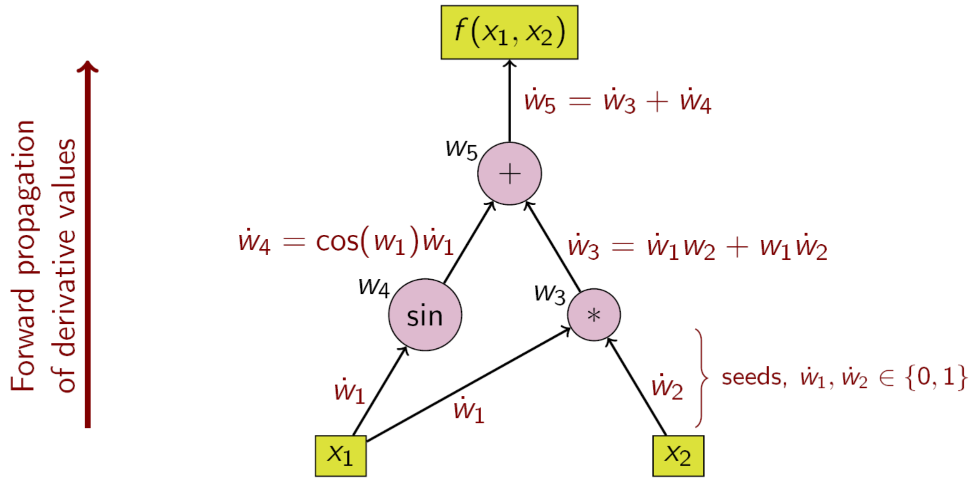
DDSim

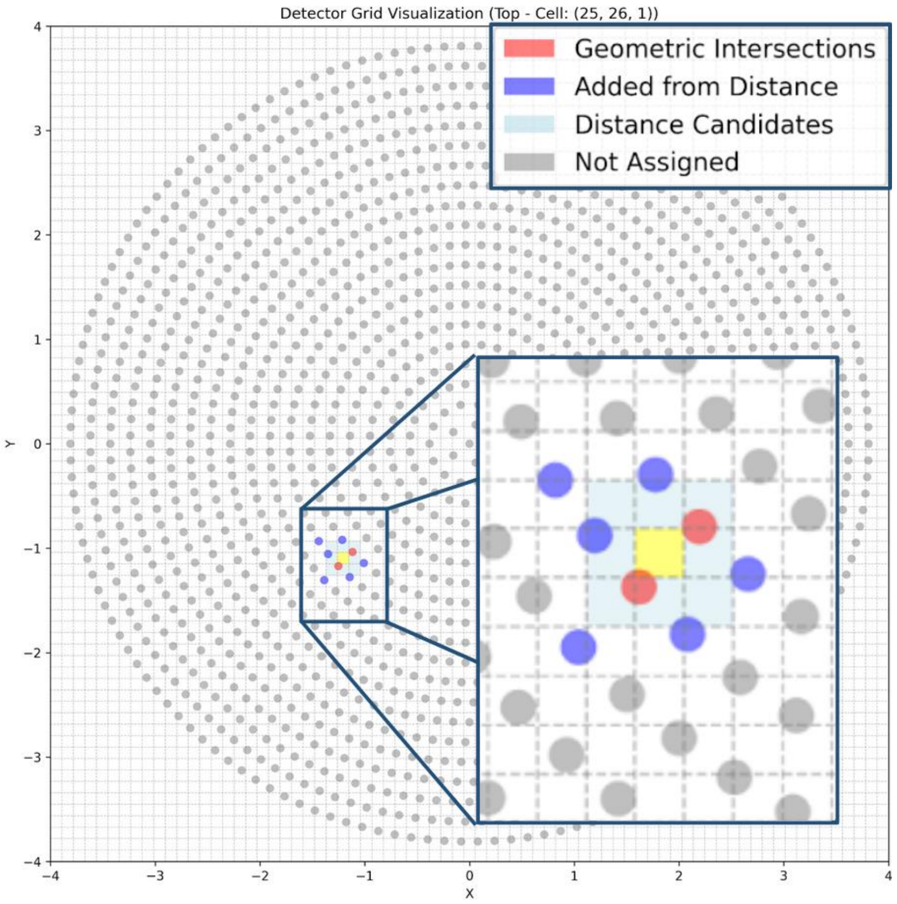
2.7% momentum resolution (assuming fixed position & direction, bias-corrected, but **charge only**), relative to:

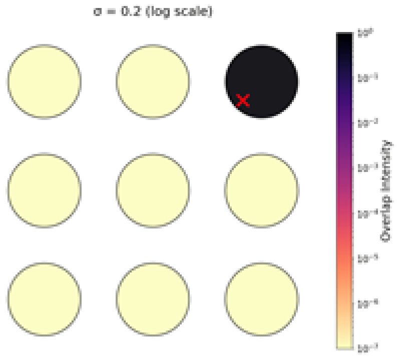
- ResNet (WatChMaL, charge+time): **2.5%**
- Traditional likelihood (fiTQun, charge+time): **~4%**

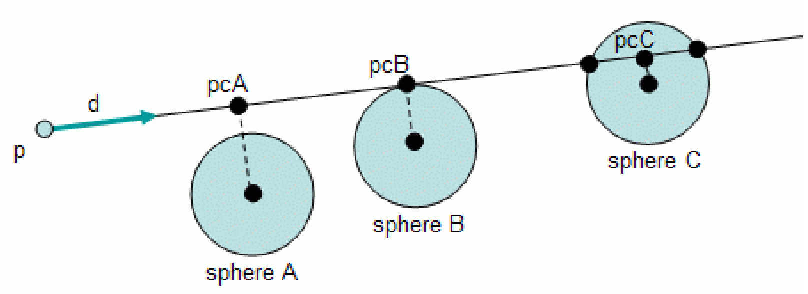
LUCID

- Light-transport Unified Calibration Inference & Differentiable detector simulation
- JAX based parallelized automatic differentiation
- Model independent ray tracing
  - Input: photon starting positions, directions, intensities
  - Find ray sphere intersection with Cylindrical grid-based acceleration structure
    - First pass: Quick check for cylinder wall or cap intersection
    - Second pass: Use grid system to identify relevant PMTs
    - Final pass: Detailed intersection calculations only for candidate PMTs
    - Acceleration from O(10k) → O(10) checks
  - Distribute photon weights based on proximity

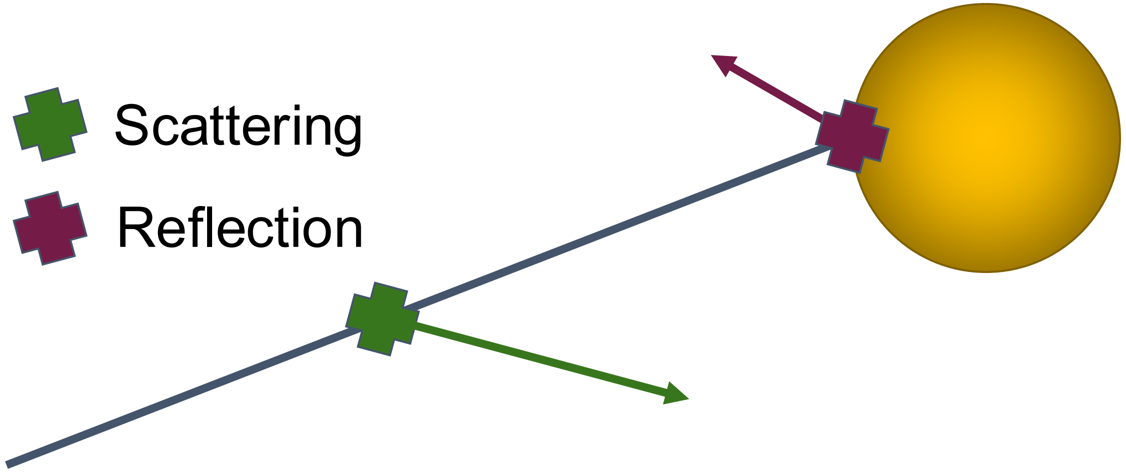




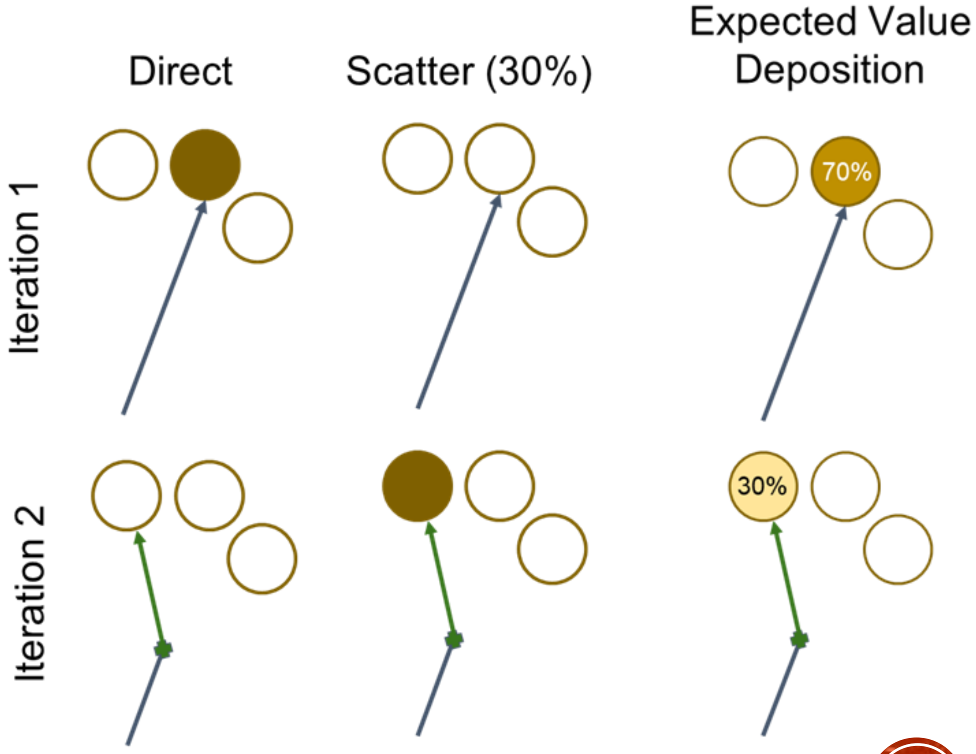




LUCID

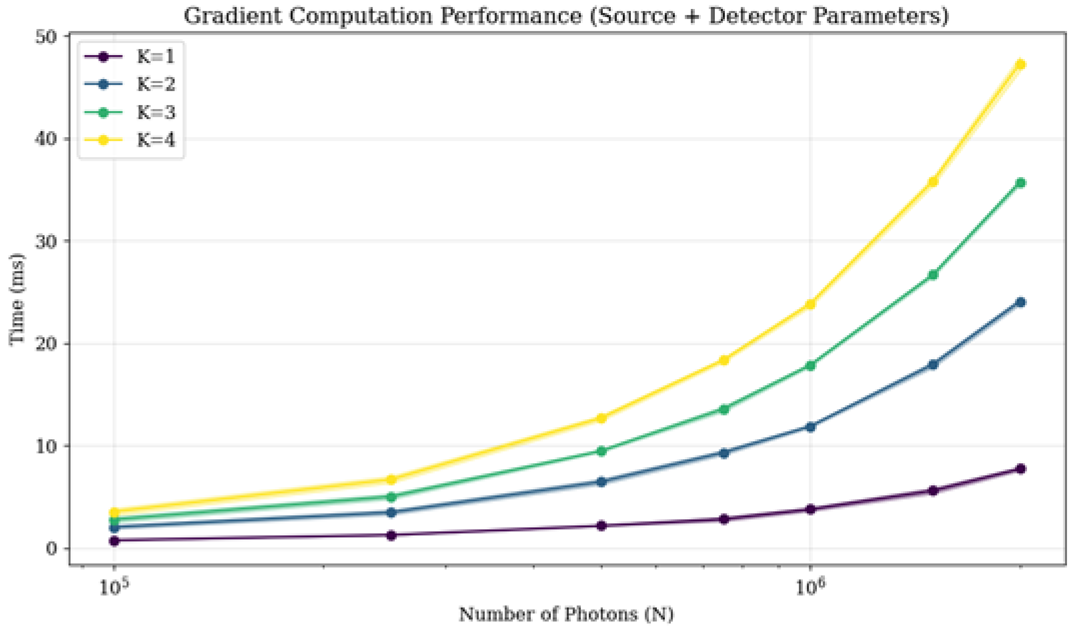


- Attenuation based on total travel distance
- Reflection and Scattering
  - Simulate N photons over K bounces (interactions)
  - Ray tracing of direct hits
  - Sampling reflection and scattering paths
    - $P\_reach = \exp(-distance/\lambda\_s)$
    - $P\_detect = P\_reach \times (1 - reflection\_rate)$
    - $P\_reflect = P\_reach \times reflection\_rate$
    - $P\_scatter = 1 - P\_reach$
    - Backward propagation with straight through estimator
    - Update intensity: $I \times (P\_reflect \times A\_reflect + P\_scatter \times A\_scatter)$

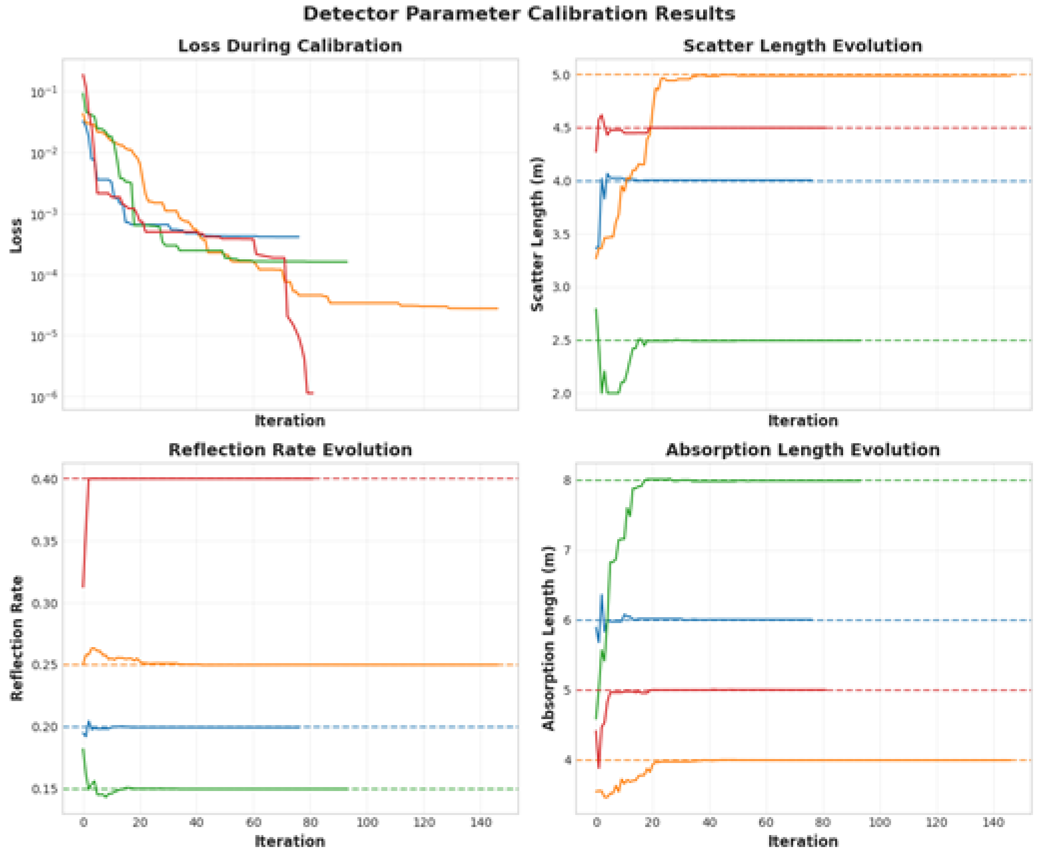


LUCID

- For K = 4 bounces on an A100 GPU, 1M photons takes:
  - 10ms for the forward
  - 25ms for forward + gradients

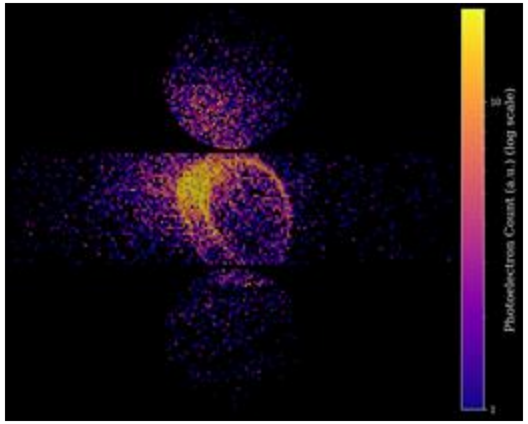


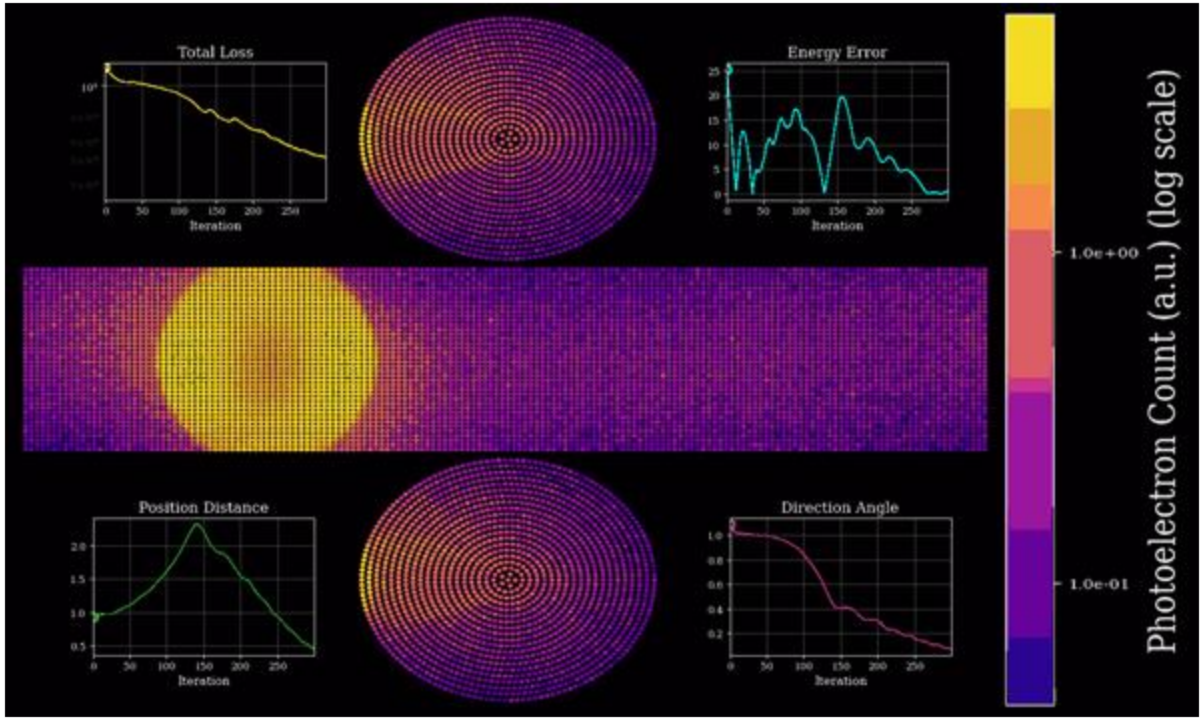
- Calibration with an isotropic photon source
  - Now testing with O(1000) PMT eff. params.

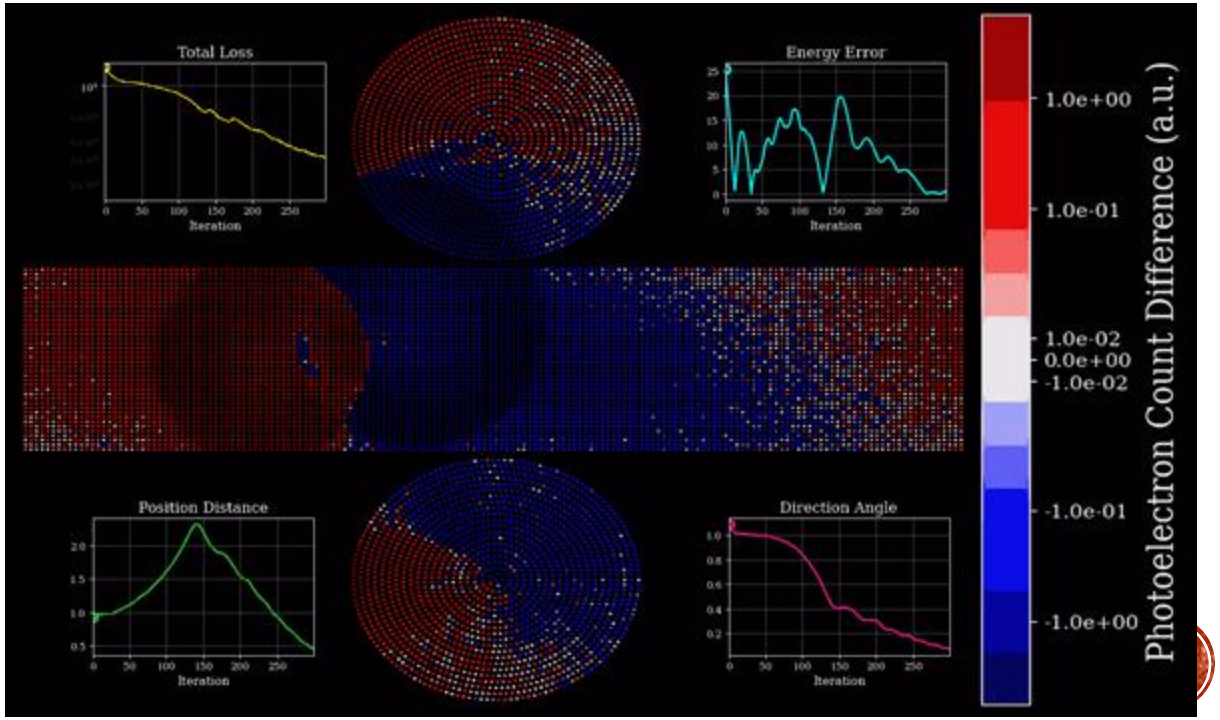


LUCID

- Connect LUCID with Cherenkov Siren
  → optimization of track parameters
- Muon full reconstruction with **LUCID**







Summary

- MC simulation requires lots of efforts to setup and tune
  - Calibration performance not ideal
  - Computation speed prohibits high statistics studies
- Future long-baseline neutrino oscillation experiments will become systematics limited
  - New near detector technologies will mitigate flux+interaction systematics
    → Reducing detector systematics becomes crucial
- Differentiable detector simulator (DDSim) proof of concept demonstrated for both water Cherenkov and liquid argon detectors
  - Already competitive performance with current traditional algorithms
- Ongoing developments to improve performance and speed of the DDSim
- Aiming for applications to real data (WCTE, DUNE ND prototypes) this FY