Advancing Detector Calibration and Event Reconstruction in Water Cherenkov Detectors through Differentiable Simulation

Omar Alterkait

Tufts University / IAIFI

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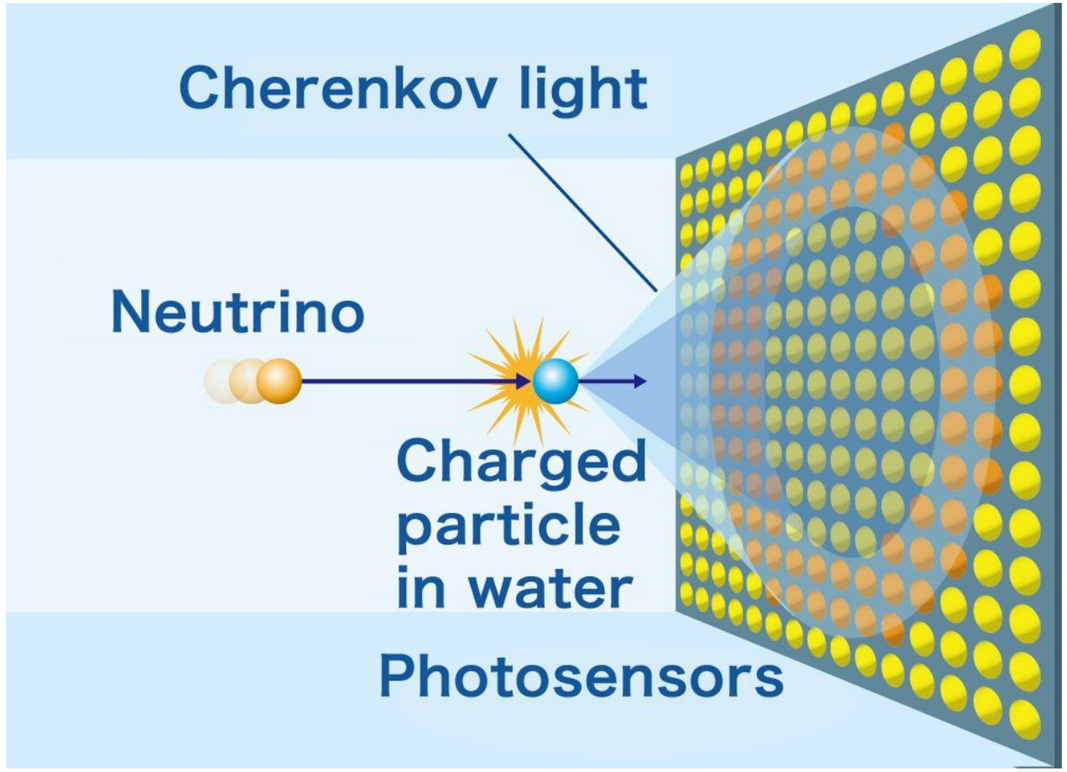
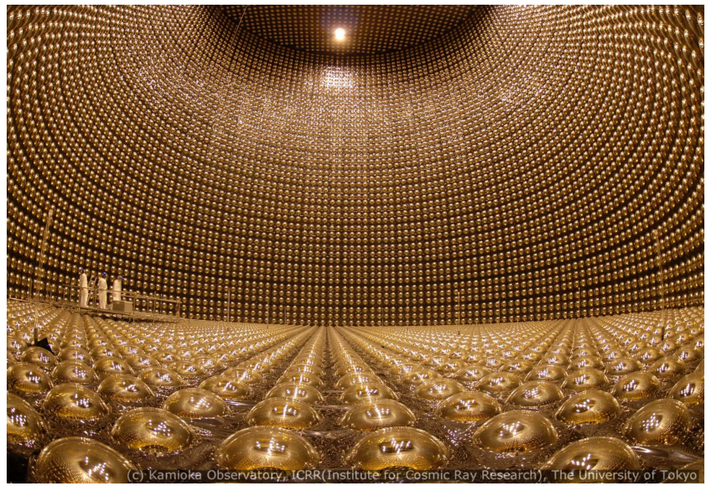
Water Cherenkov Detectors

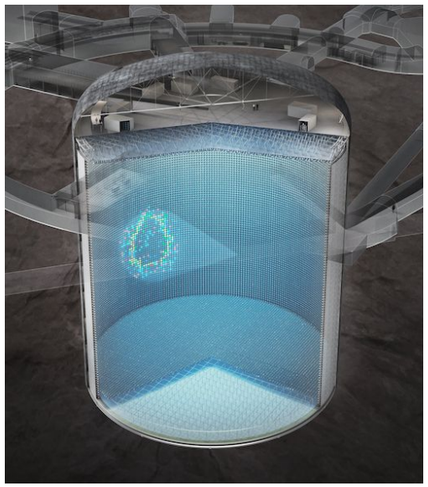


- Cones of cherenkov light emitted when particles exceed light speed in water
- Thousands of photosensors line detector walls to capture faint light signals

- Super-K: 50 kiloton detector that transformed our understanding of neutrinos
- Hyper-K: Massive 260 kiloton facility targeting transformative discoveries across the neutrino sector
- Calibration techniques must evolve to match increased detector scale and enable the precision required new discoveries



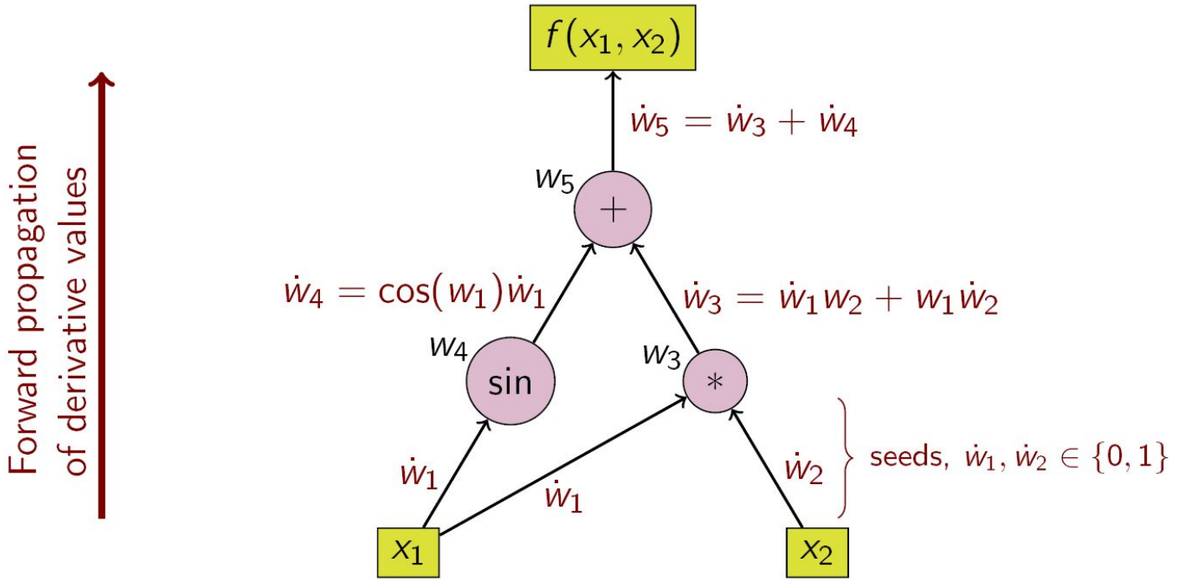
Super Kamiokande



Hyper Kamiokande

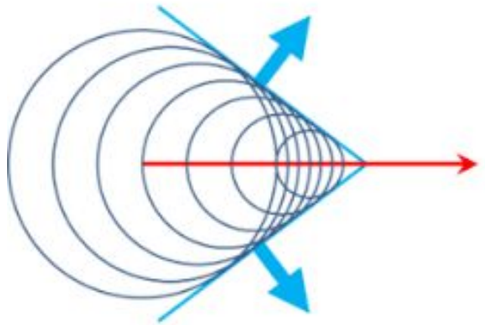
Automatic Differentiation to the Rescue

- Automatic Differentiation (AD): Computes exact partial derivatives through the chain rule by tracking operations
- Provides machine-precision exact gradients
- Chose JAX to be the AD framework
- JAX advantages: GPU acceleration, vectorization, JIT compilation
- 100-1000× speed improvement on GPUs O(10ms) full simulation



$$
\begin{aligned}
y &= f(x_1, x_2) \\
&= x_1 x_2 + \sin x_1 \\
&= w_1 w_2 + \sin w_1 \\
&= w_3 + w_4 \\
&= w_5
\end{aligned}
$$

Cherenkov Profiles

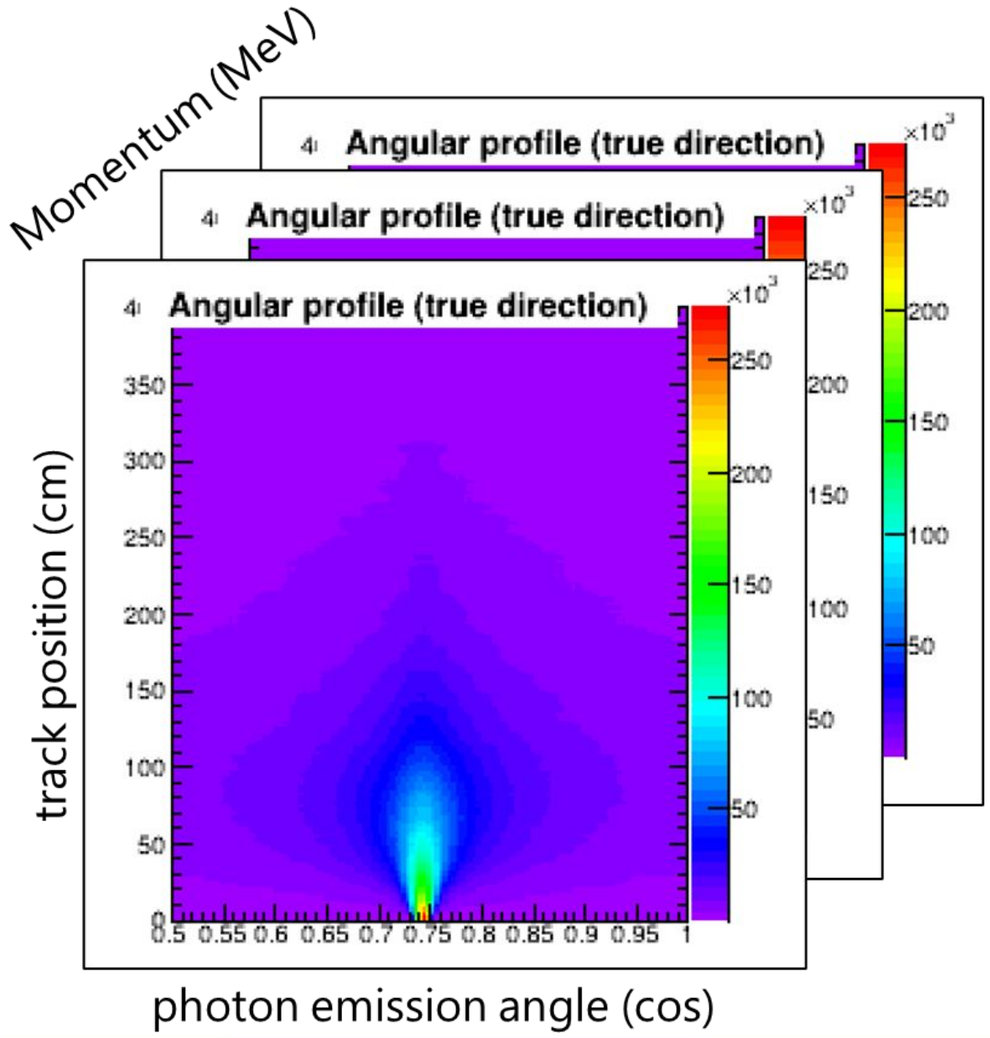


Generate Photons

Propagate Photons

- Cherenkov Profiles: 3D histograms incorporating particle physics from momentum to photon generation

- SIREN Neural Network Implementation:
  - Inputs: momentum, emission angle, track position
  - Output: photon intensity at specified location - Enables differentiable sampling along particle paths



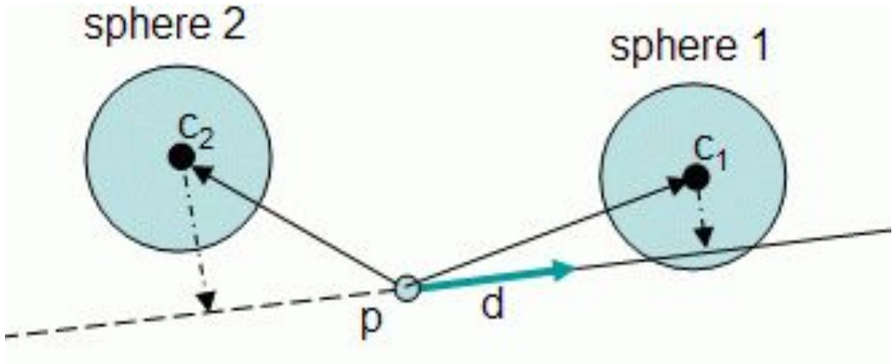
Ray Tracing

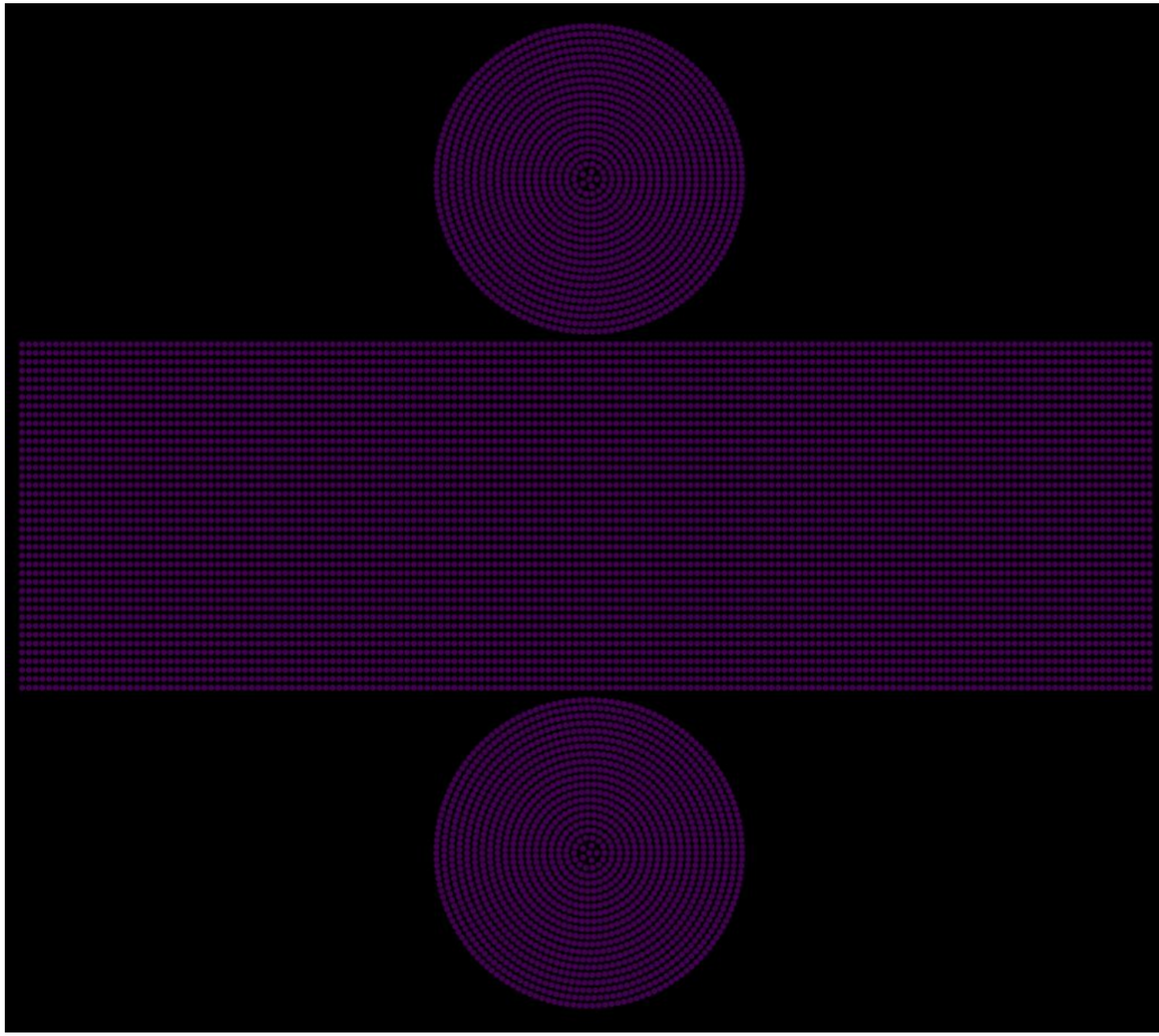
Generate Photons

Propagate Photons

The biggest bottleneck by far in the detector simulation is the ray tracing.

The detectors are assumed to line up the walls and caps of a cylinder. We can use ray sphere intersection to find the final location each ray





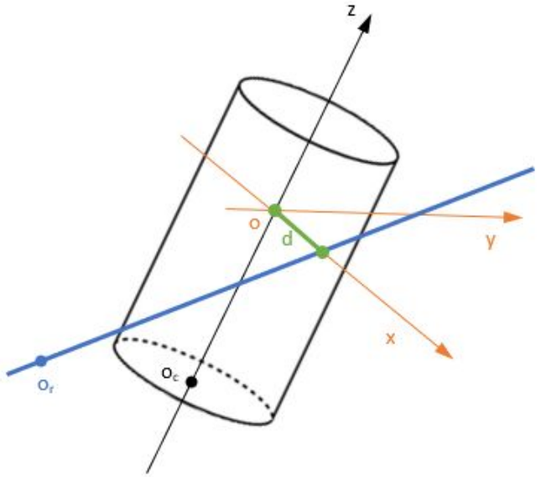
Smart Intersection Detection

Generate Photons

Propagate Photons

Let's make our simulation faster:

- Checking every PMT for each photon is computationally wasteful
- Key insight: We can pre-filter likely intersections
- Solution: Cylindrical grid-based acceleration structure

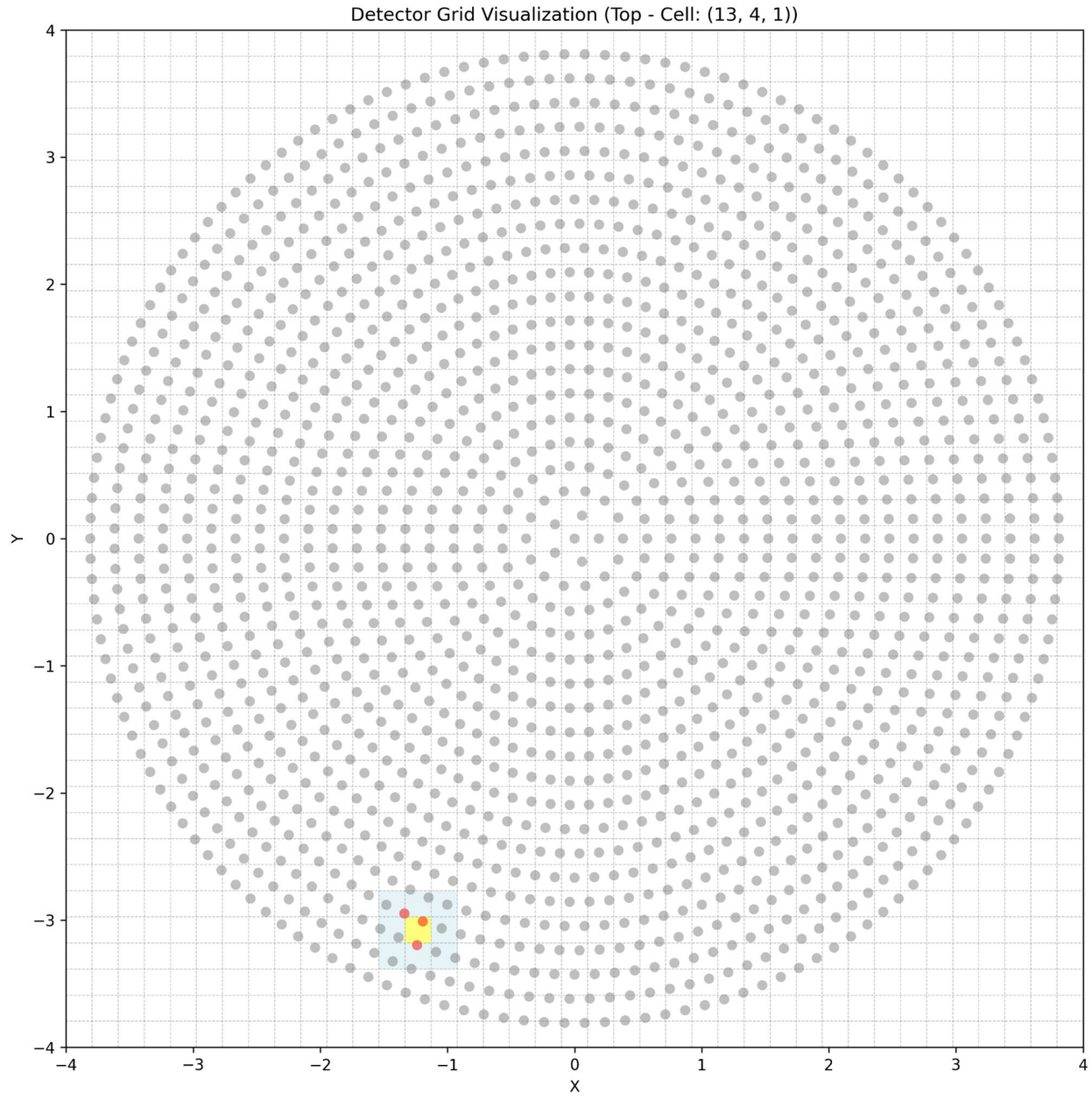


Our approach:

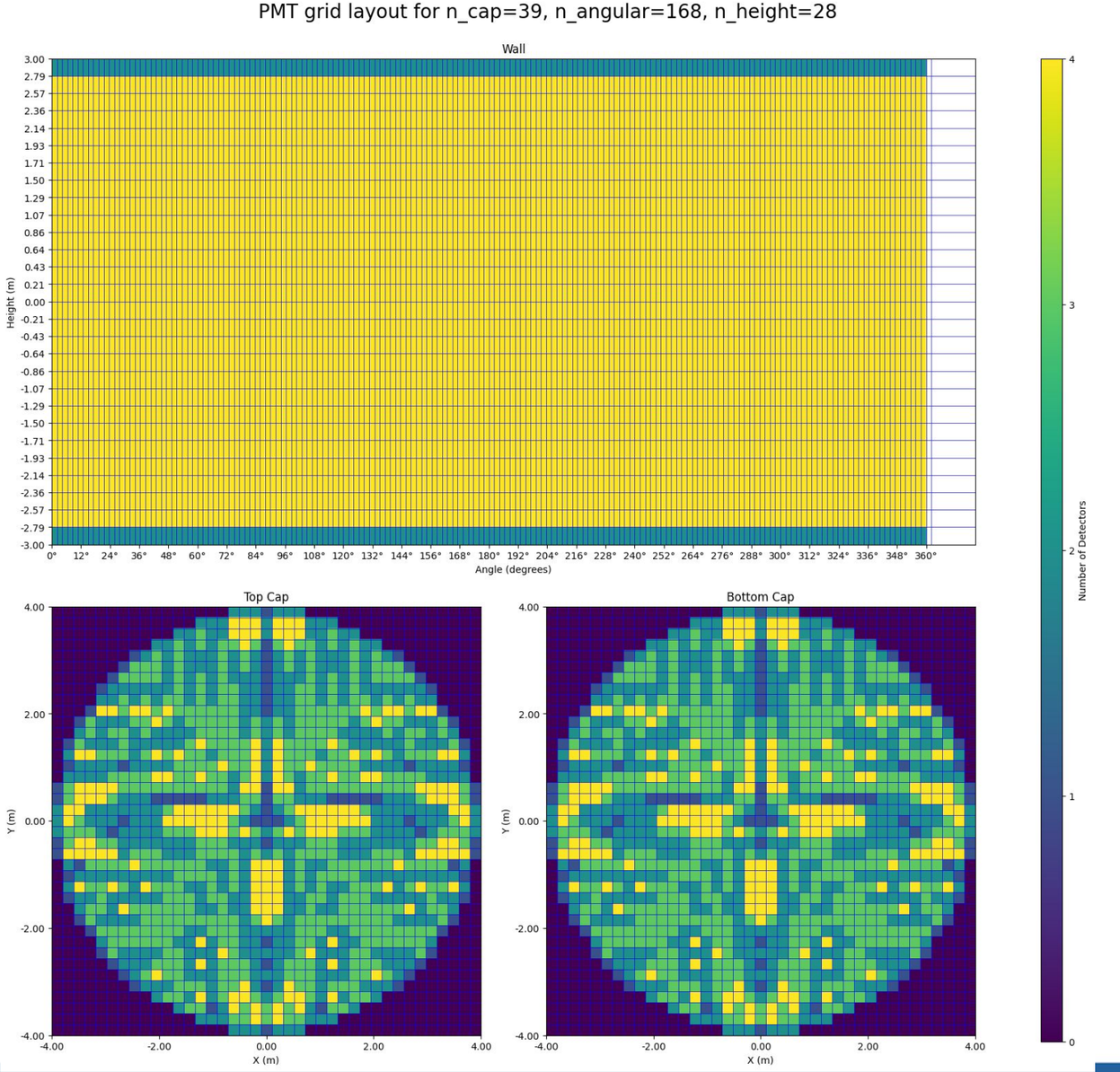
1. First pass: Quick check for cylinder wall or cap intersection
2. Second pass: Use grid system to identify relevant PMTs
3. Final pass: Detailed intersection calculations only for candidate PMTs

The grid system is extremely efficient given simple division and floor operations

Detector Grids



Number of PMTs per grid



From Discrete to Continuous Detection

Generate Photons

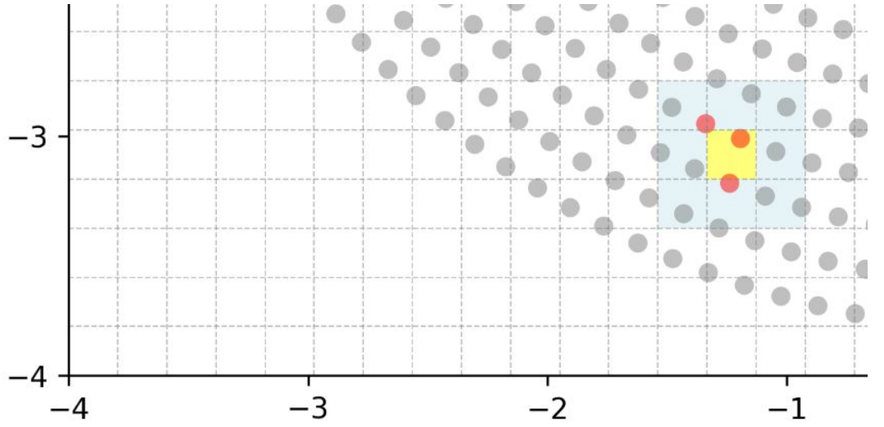
Propagate Photons

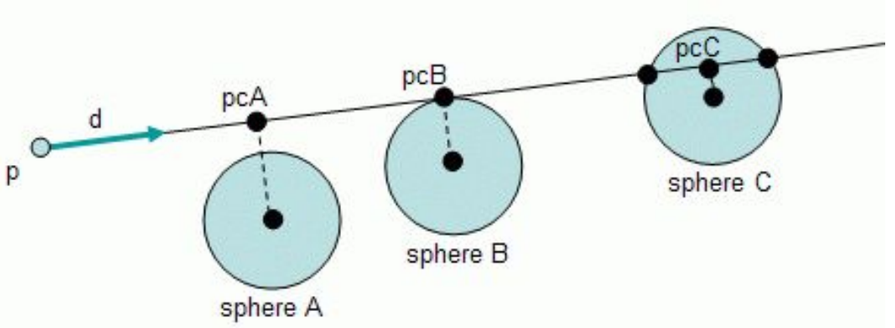
Traditional ray tracing problem: photons either hit or miss PMTs completely.

Our approach:

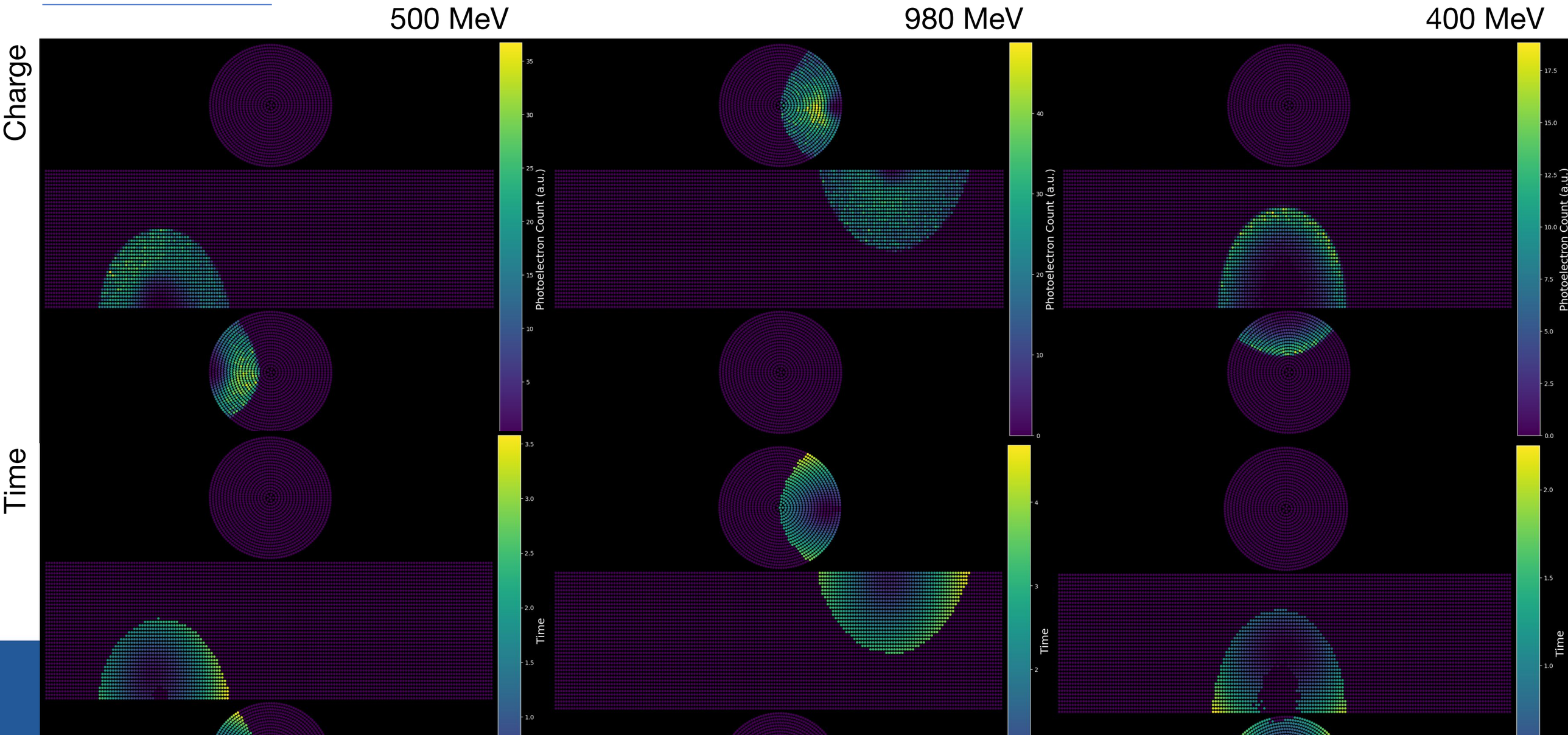
- Replace hard binary decisions with smooth probability weights
- Calculate weights based on proximity between photon path and PMT
- Adjust sensitivity through a tunable temperature parameter

This approach creates smoother gradients and significantly reduces optimization noise



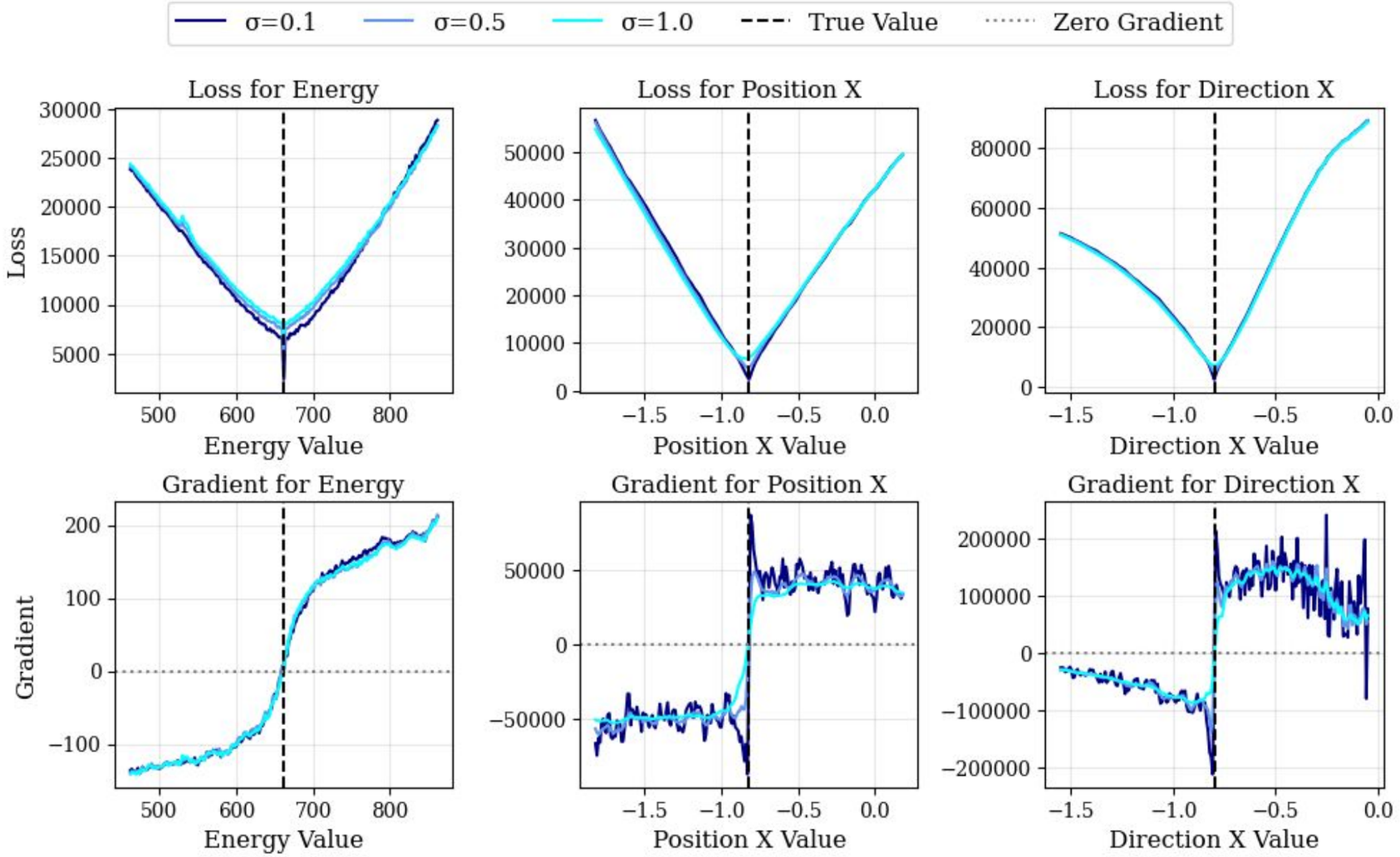


Event Displays



One Parameter Gradients

- The first sanity check we can do, is freeze all parameters of the simulation, and alter one at a time.
- Reconstruction Parameters:
  - Energy
  - 3D Position
  - Direction (represented as a 3D vector)

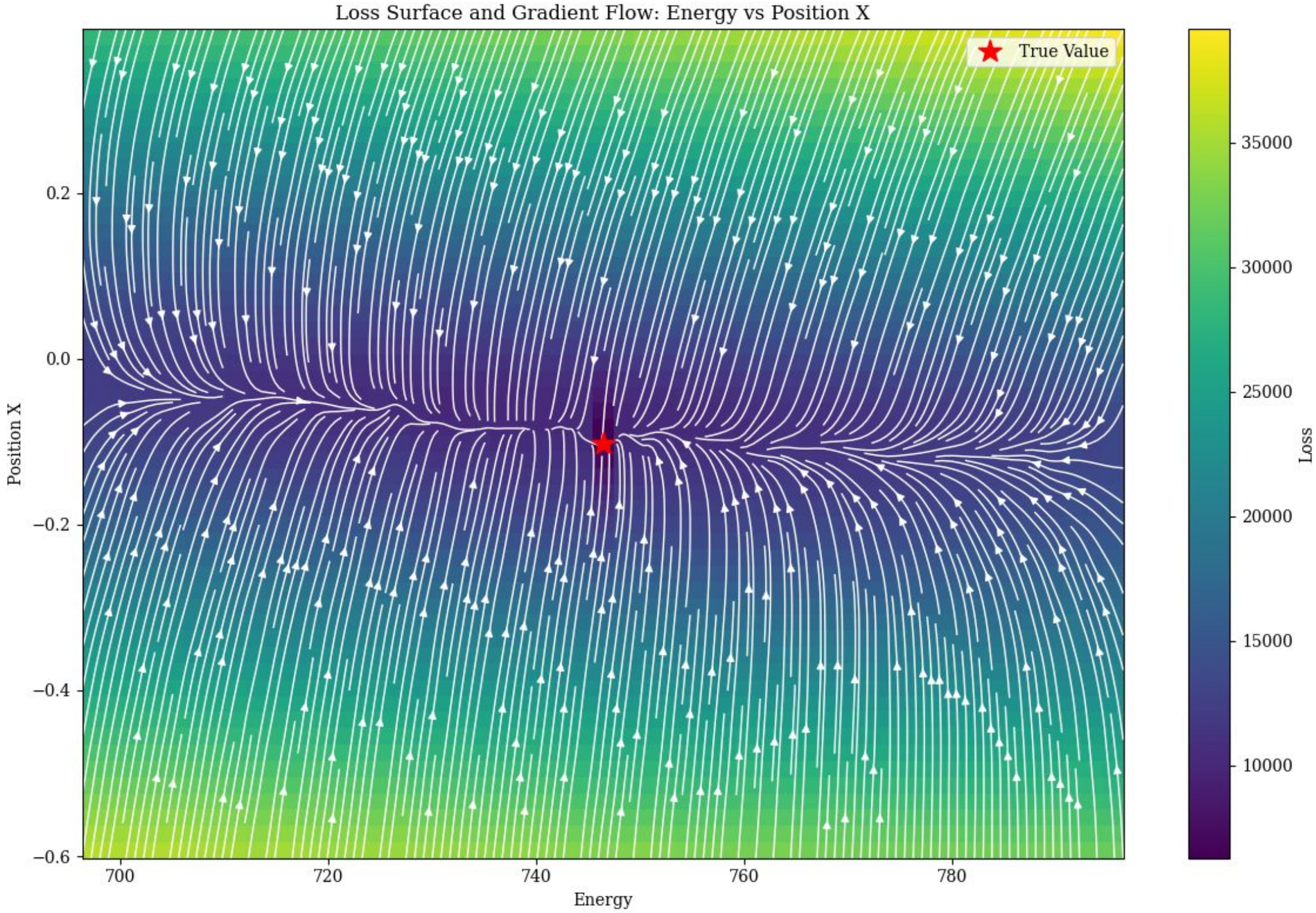


2 Parameter Variation

We can vary two parameters and look at the gradients extracted. The color is the loss.

The streamlines are the values of gradients at those locations

Energy/Position



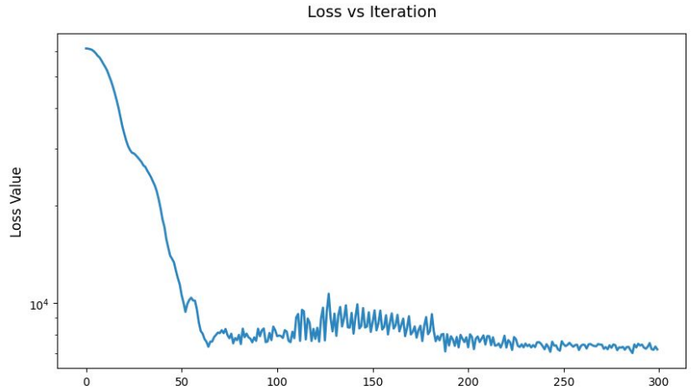
Training Results

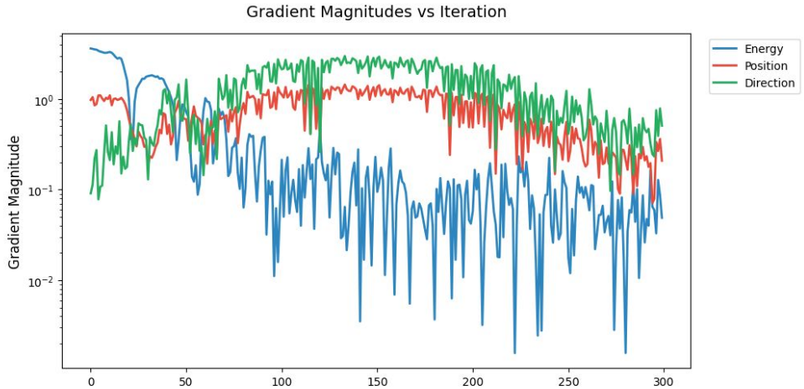
Difference in Parameters True vs Simulation:

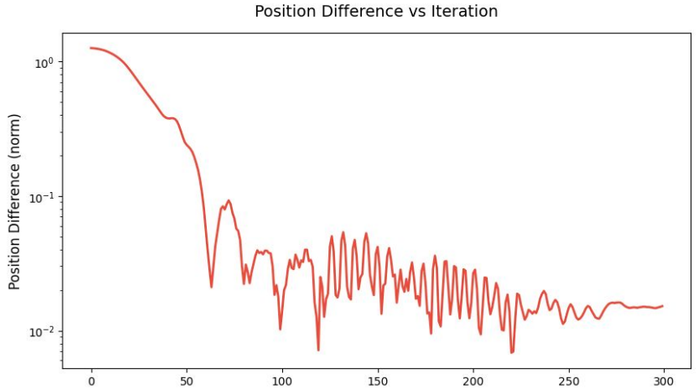
Energy: -4.14 MeV
Percent: 0.59 % (700 MeV)

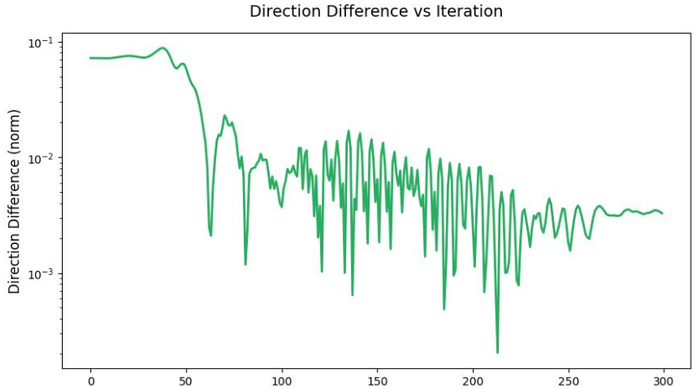
Position: 0.015 ,
difference/pmt_radius: 0.379

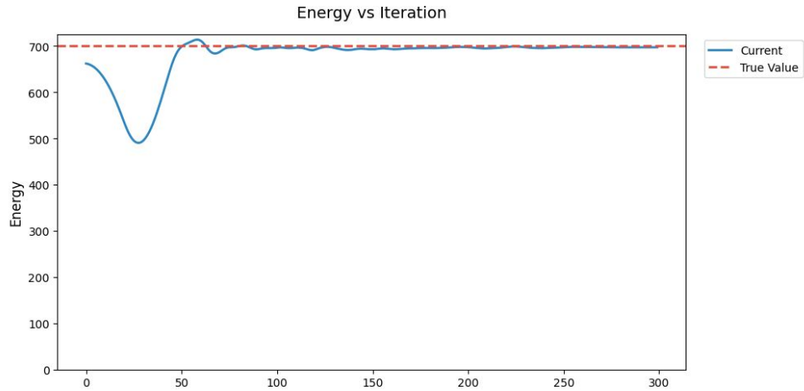
Direction: 0.0032 ,
Angular: 0.186 degrees

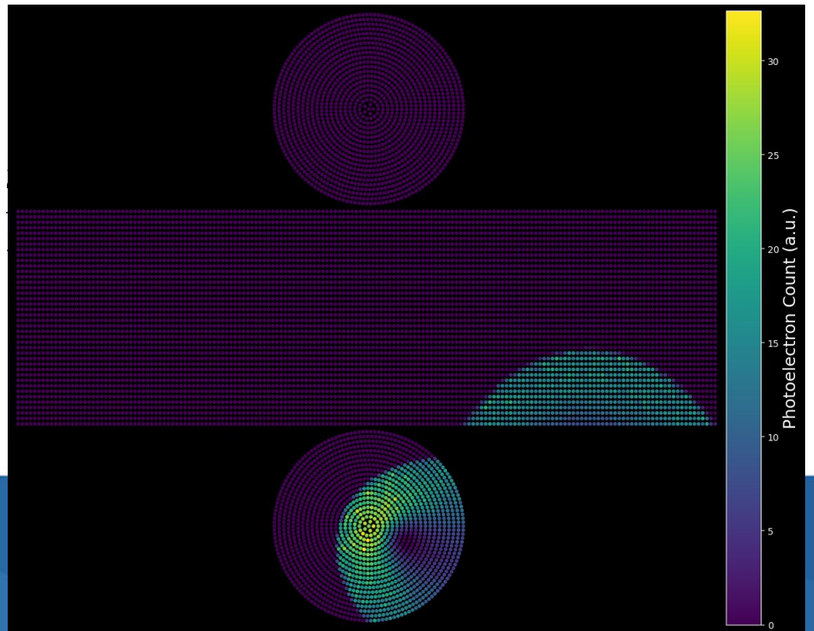












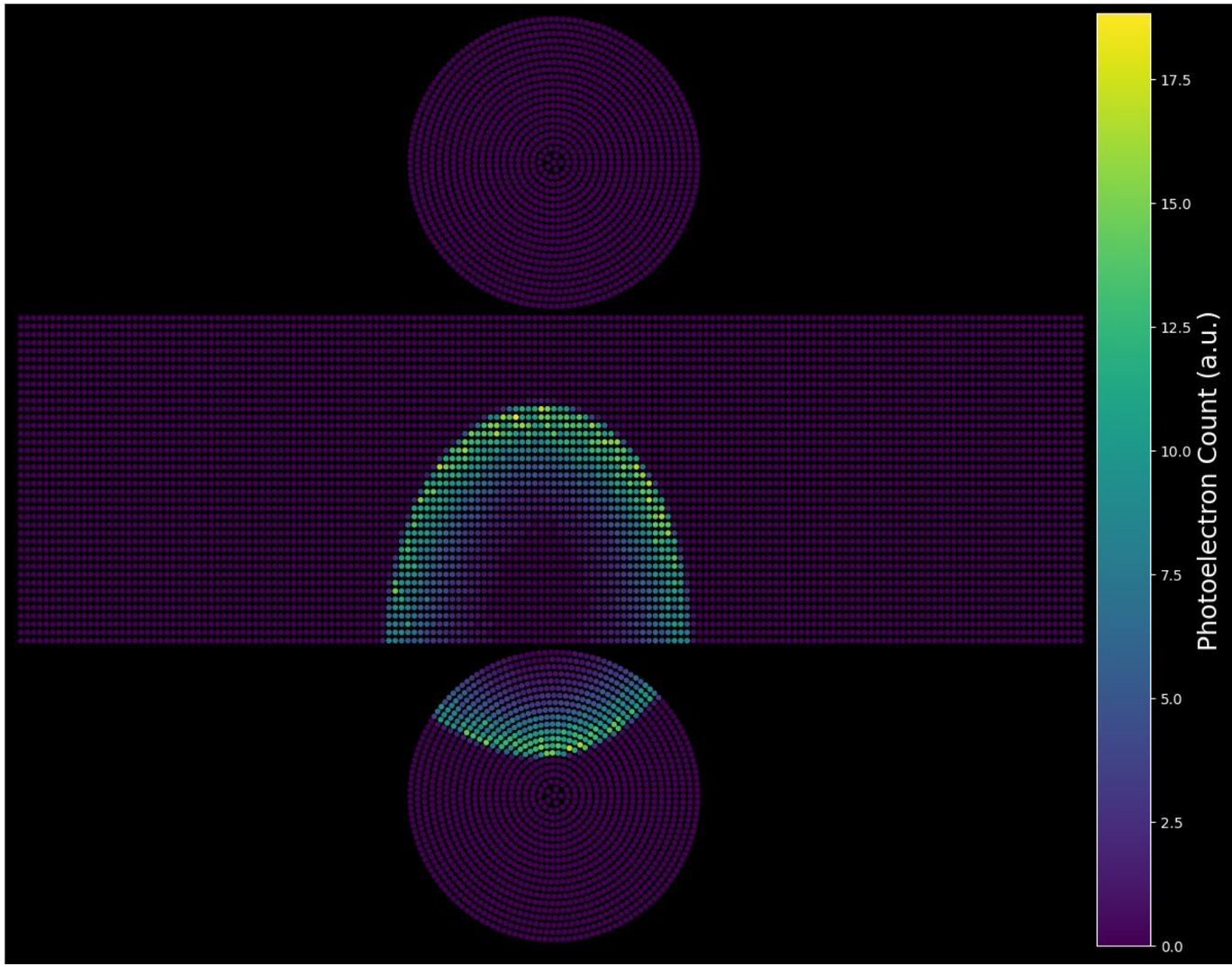
Conclusion

Our differentiable simulation offers:

- Rich gradient information for reconstruction and calibration
- Physically interpretable results compared to NNs

Next Steps:

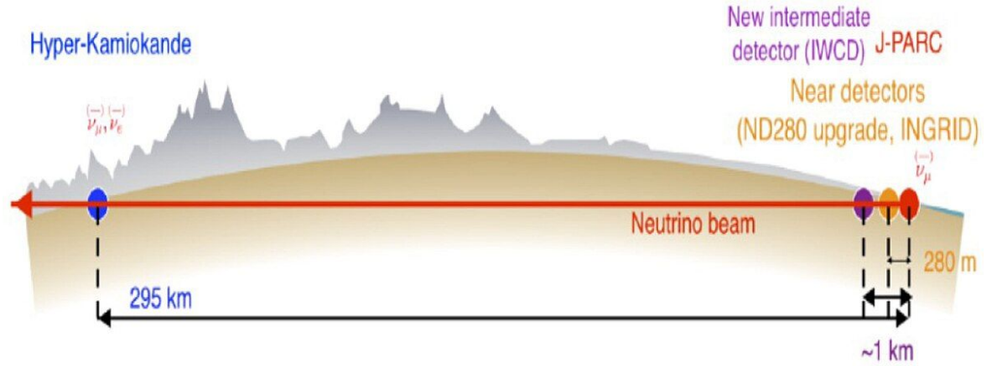
- Include Stochasticity through reflections and scattering
- Employ a more realistic geometry

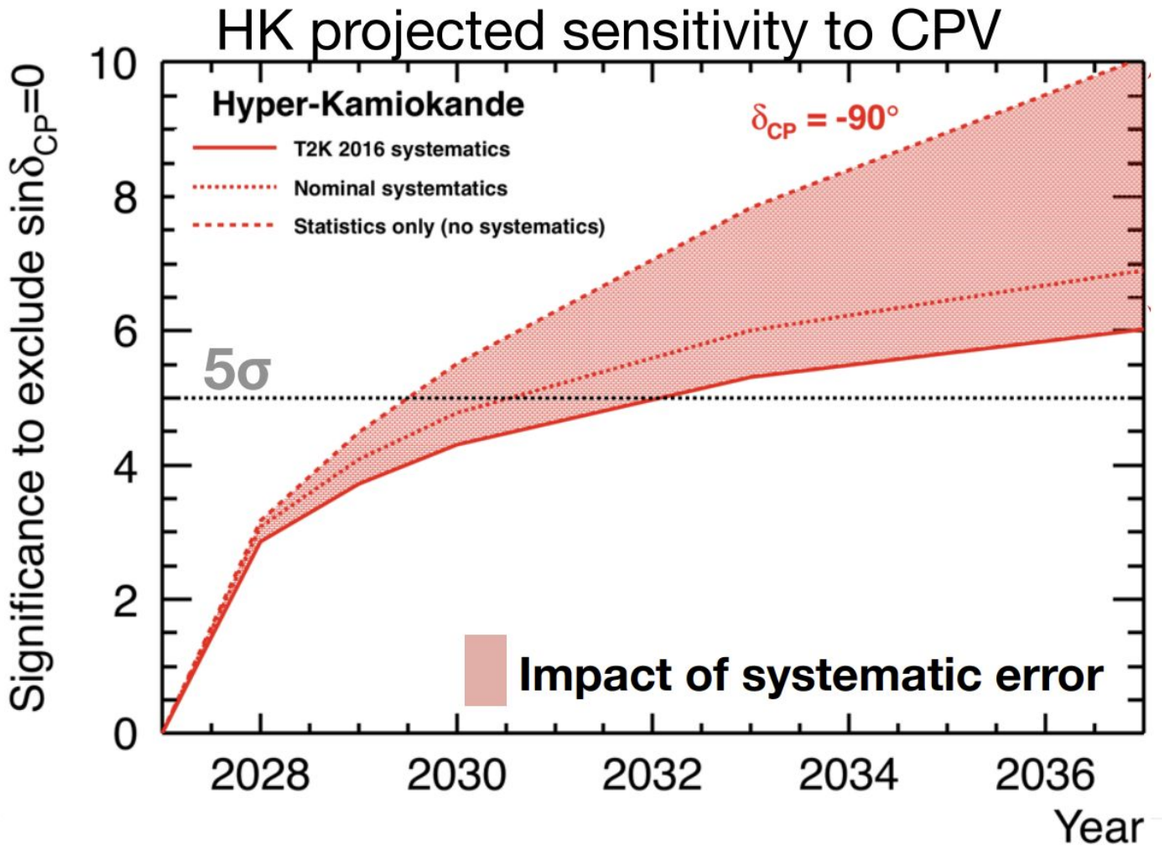


Backup

Precision Era of Neutrino Oscillation Measurements

- CP violation in neutrinos remains a fundamental open question in particle physics
- Hyper-K and next-generation experiments designed to definitively resolve the CPV question
- Plot demonstrates how systematic uncertainties directly impact discovery timeline by 2-3 years
- Reducing systematics requires innovative techniques in detector calibration and reconstruction

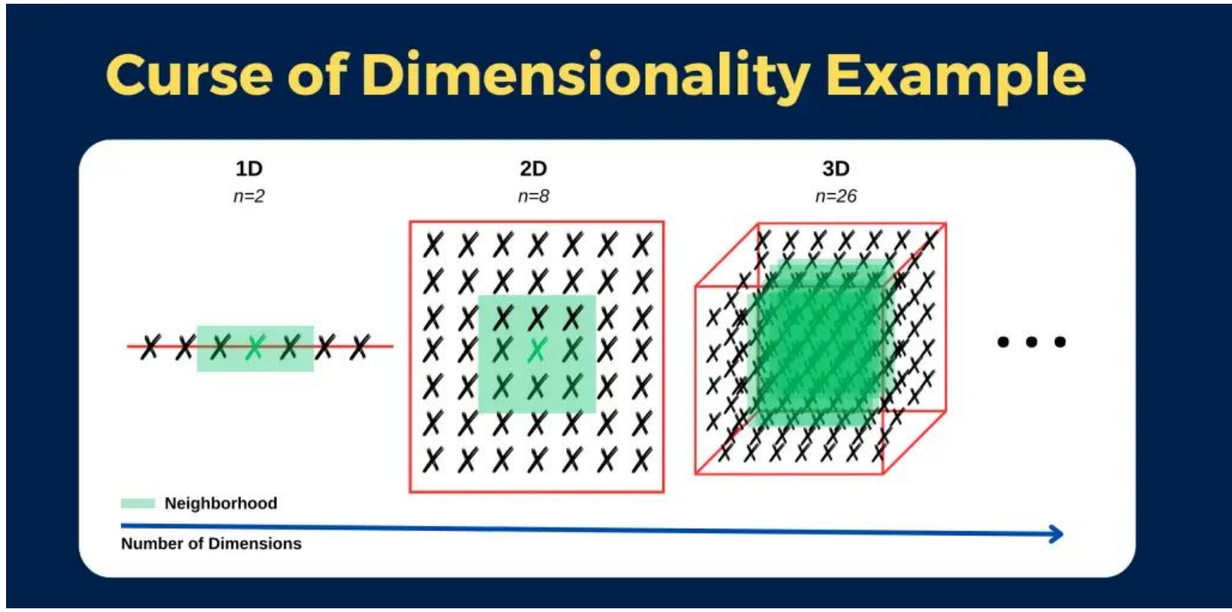




Hyper-K DR: arXiv1805.04163

Curse of Dimensionality

- Detector response depends on: optical properties, PMT characteristics, medium properties, geometry factors...
- Full calibration requires many independent parameters
- Grid search scales as O(N^d) → evaluations become computationally infeasible without simplifying approximations
- Numerical gradient methods: unstable in complex optical models, prone to local minima



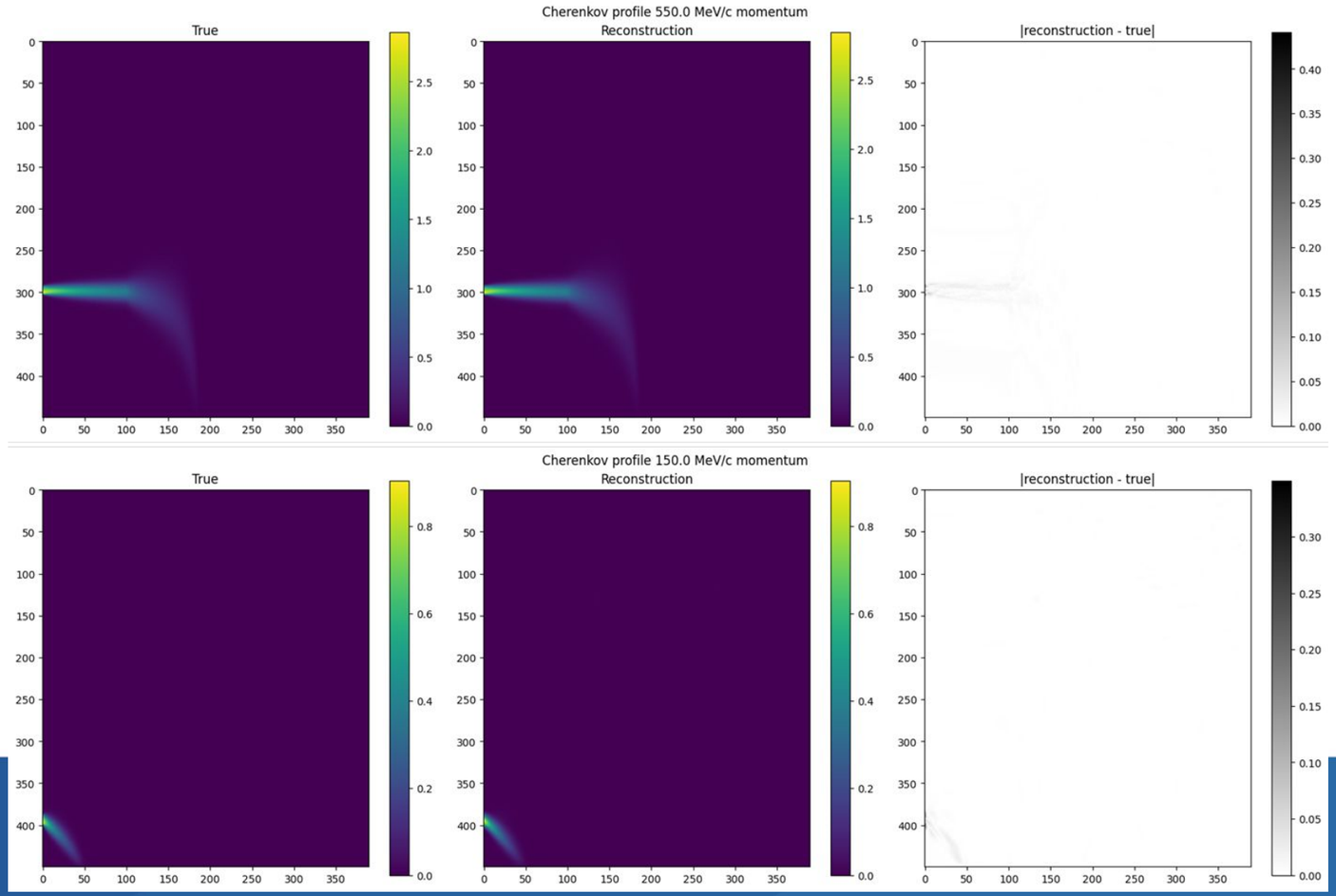
CherenkovSiren (work in progress)

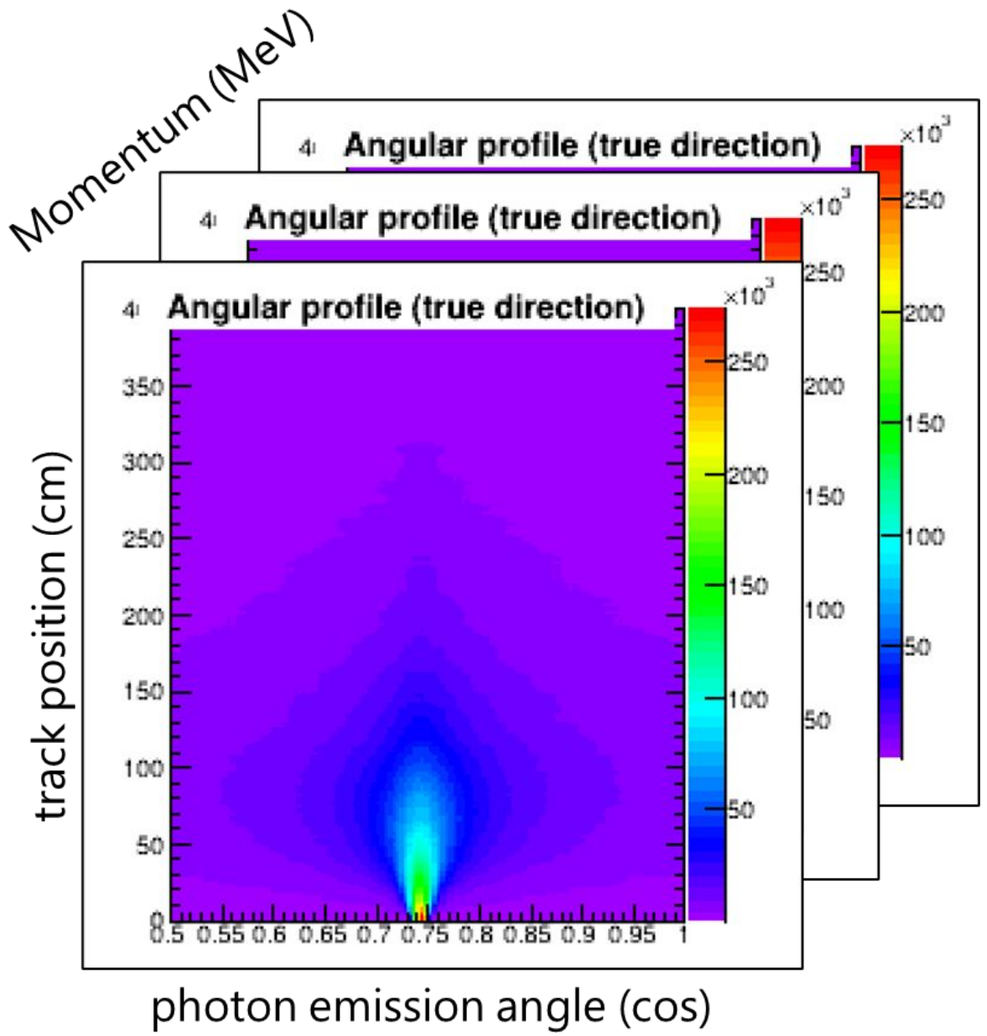
Generate Photons

Propagate Photons

Detect Photons / PMT Hit

- Trained CherenkovSiren Models:





Photon Relaxation: Gaussians

Proposed Solution:

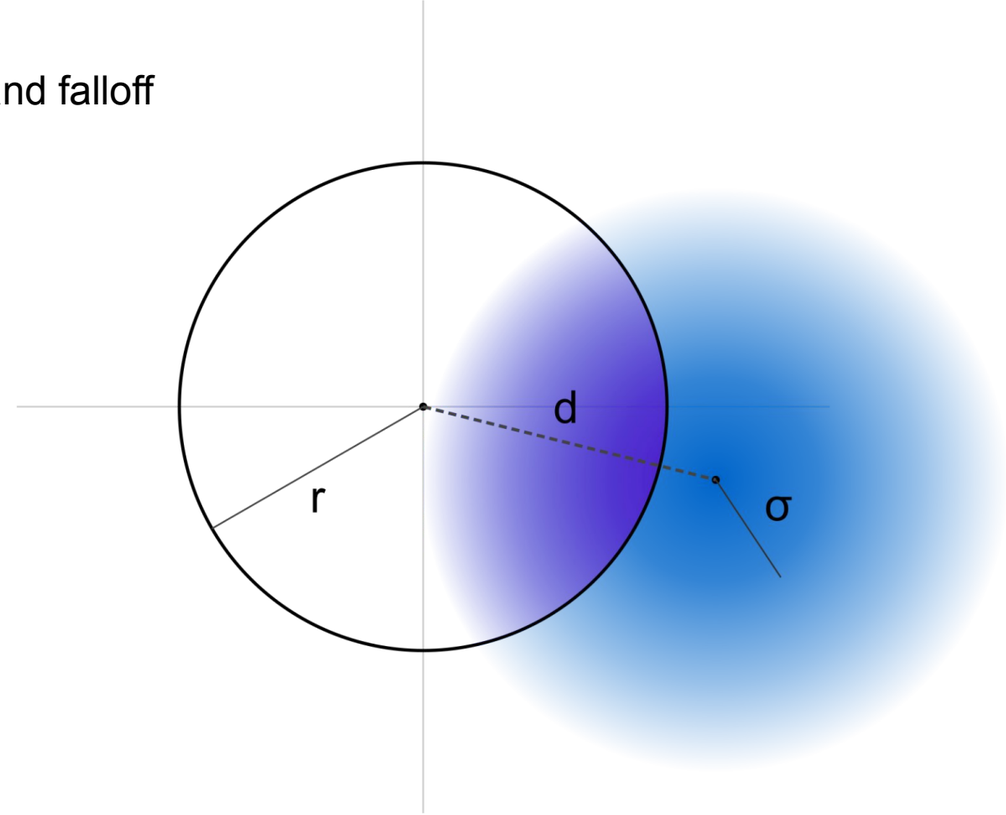
- Model the “contribution” to each PMT as the photon overlapping with a circular detector on the wall
- Represent photons as distributions with spatial falloff
- Requires precise calculation of 2D overlap integral between the circle and falloff

Integration Challenge:

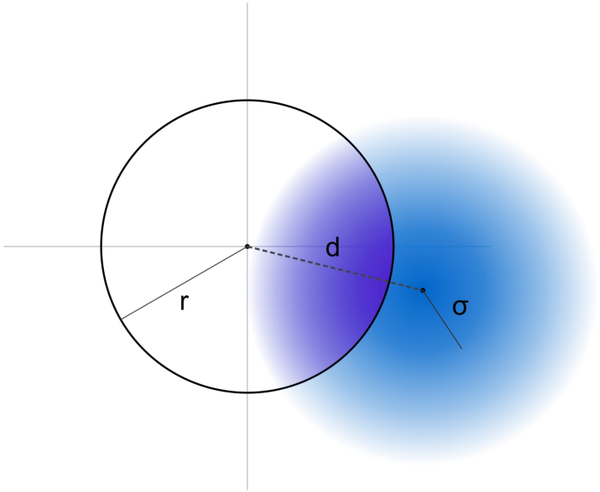
- Full 2D overlap integral needed
- Parameters: PMT radius (r) and distribution width (sigma)

Optimization Strategy:

- Leverage problem symmetry
- Pre-calculate overlap as function of distance (d)
- Distance measured to closest point on trajectory
- Reduces computational overhead significantly



Overlap Calculation



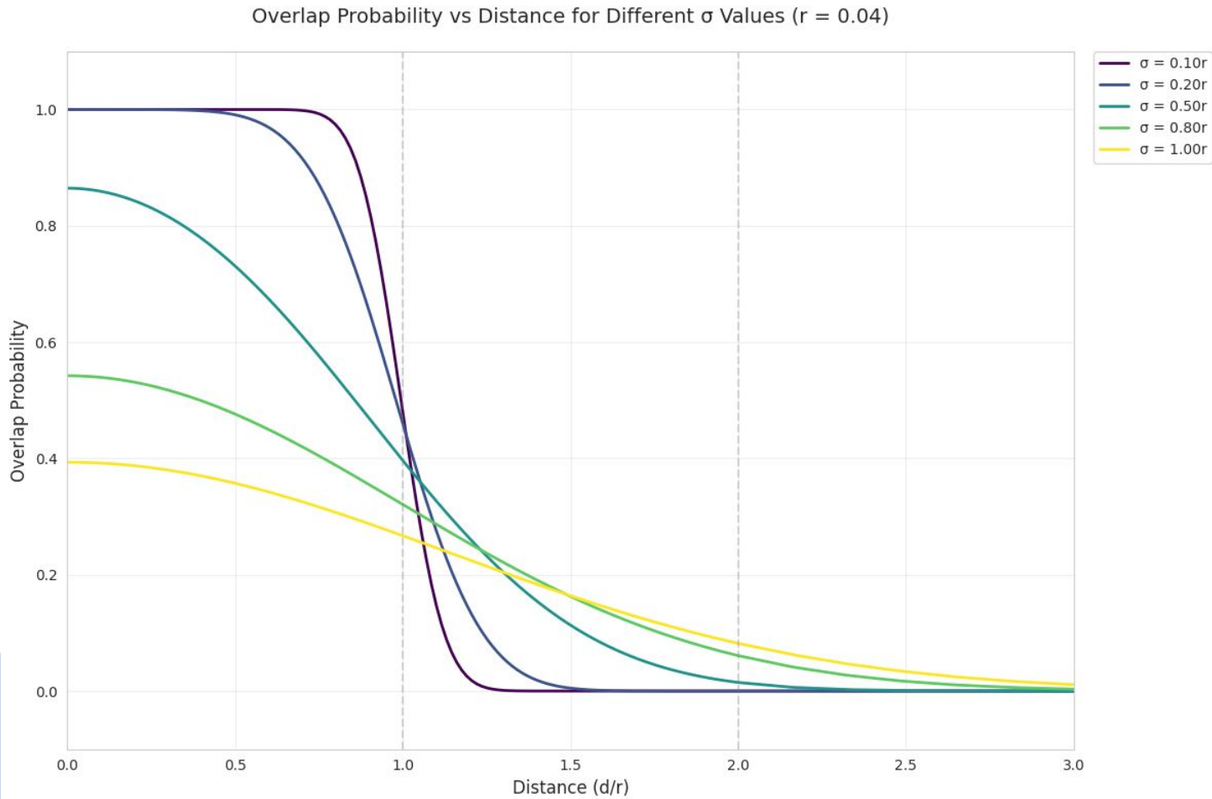
1D differentiable lookup table in JAX.

Save the overlap values and the gradient at that location and interpolates between them

Overlap Probability Values at Selected Distances:

Overlap Probability Values at Selected Distances:

σ	d = 0	d = 2r	d = 3r	d = 4r
0.10r	1	5.37e-24	0	0
0.20r	1	1.99e-07	1.07e-23	0
0.50r	0.865	0.0147	1.87e-05	6.18e-10
0.80r	0.542	0.0609	0.00322	4.28e-05
1.00r	0.393	0.0819	0.0109	0.000604



Realistic PMT Simulation

Generate Photons | Propagate Photons | **Detect Photons / PMT Hit**

From photons to signals:

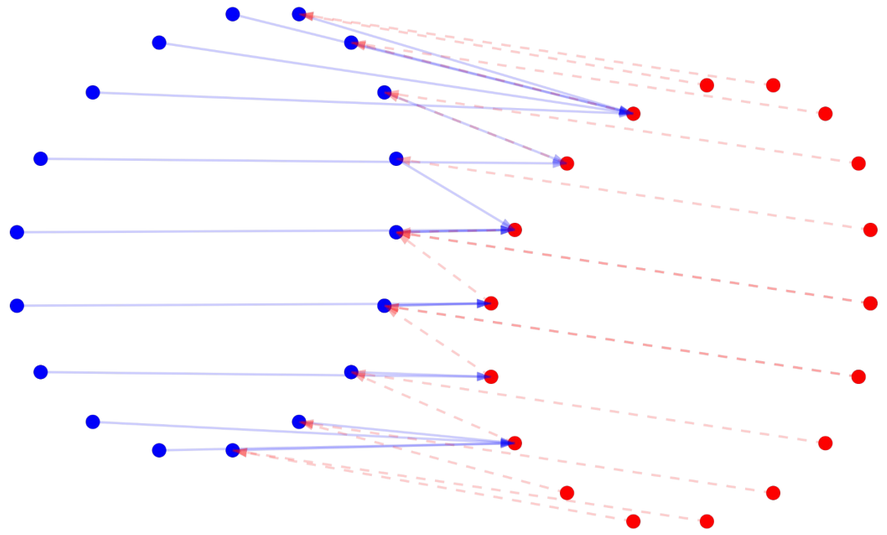
- Accumulate weighted contributions per PMT
- Calculate charge and arrival times to obtain hits
- Framework easily extendable for PMT response:
  - Angular acceptance
  - Quantum efficiency
  - Time response

Future capabilities:

- Train response models on calibration data
- Fine-tune using real detector data

Loss Construction

- Loss = Metric comparing how well simulation matches data that we would like to minimize
- Finding closest PMT pairs between sim/data:
  - Need differentiable matching between active PMTs
  - Use softmin weighted by distance parameter τ
  - Smooth approximation instead of direct minimum
- Time alignment:
  - Remove mean time from sim and data
  - Accounts for unknown t0 offsets
- Combined loss components:
  - L_charge: Compare charge ratios of matched pairs
  - L_time: Compare aligned timing differences
  - Total Loss = L_charge + λ L_time



Bringing It All Together

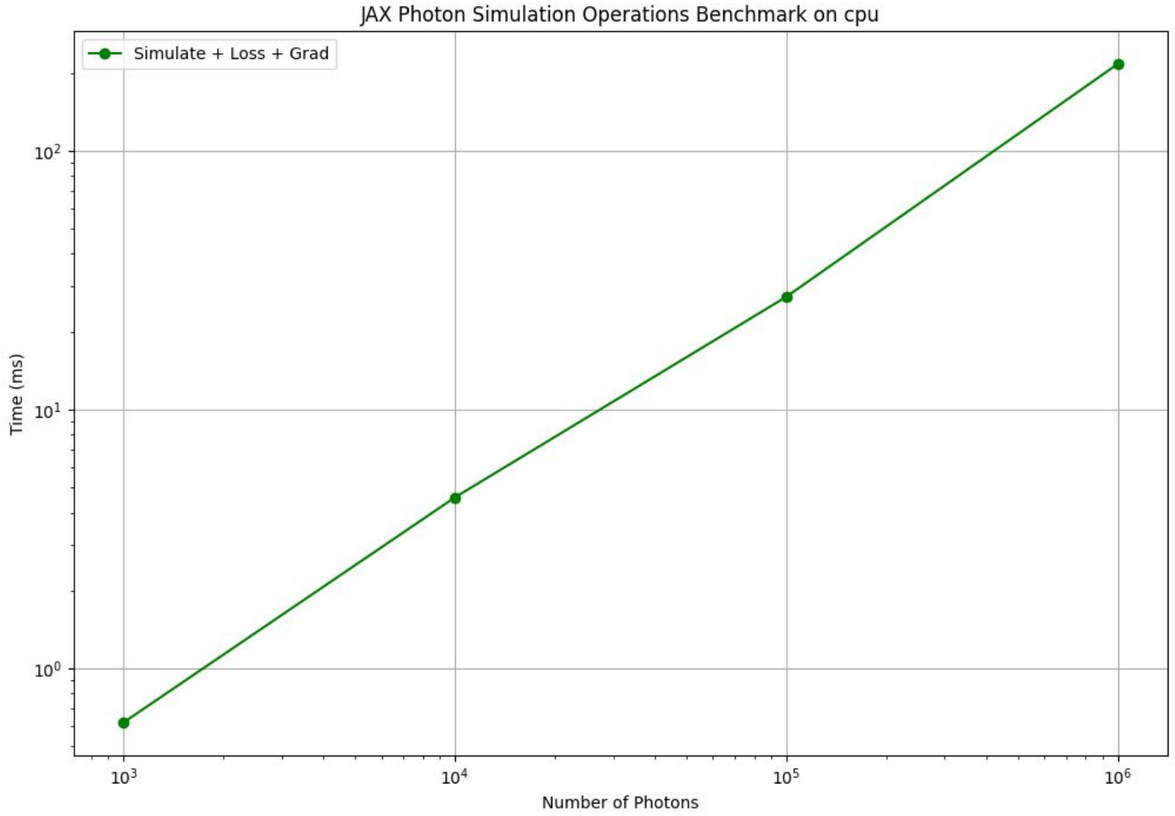
Complete differentiable simulation pipeline:

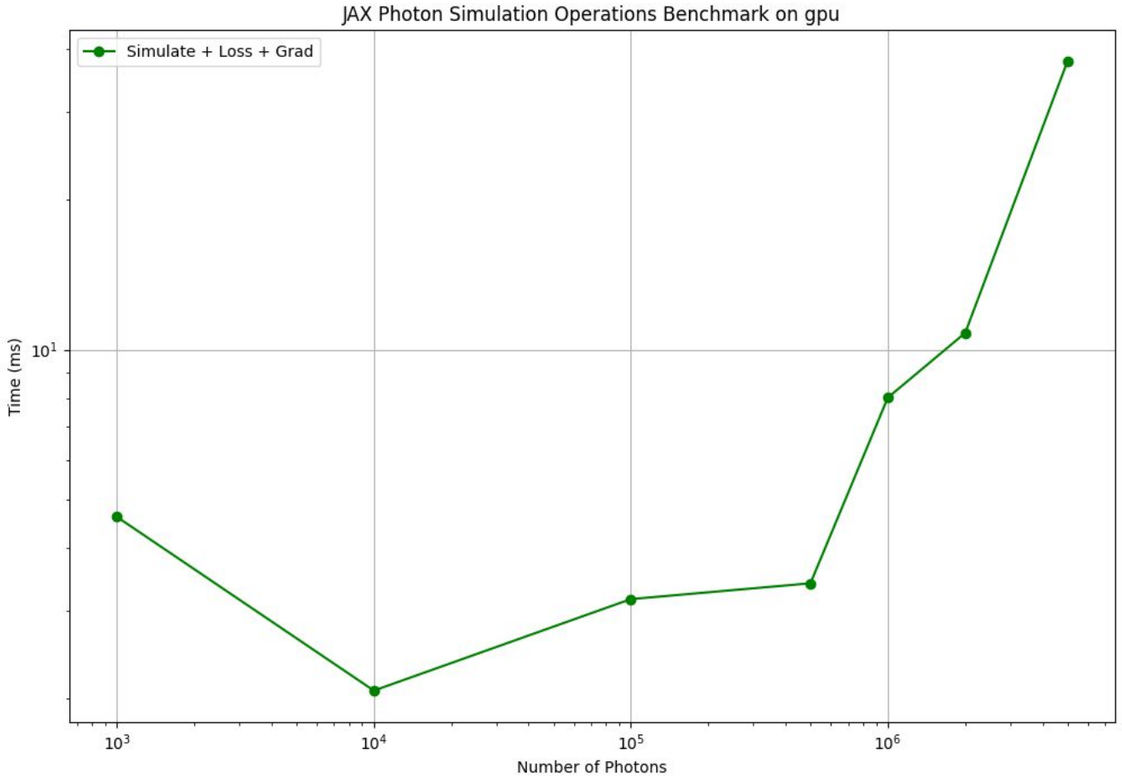
1. Generate initial parameter guess
2. Compare simulation to real data:
    - PMT charge differences
    - Normalized timing differences (time - mean_time) / std_time
3. Compute gradients automatically
4. Update all parameters simultaneously

Key advantage: Single backward pass gives gradients for ALL parameters

Speed (without CherenkovSiren)

on a 4090 GPU, 1M photons takes 8 ms for the full cycle





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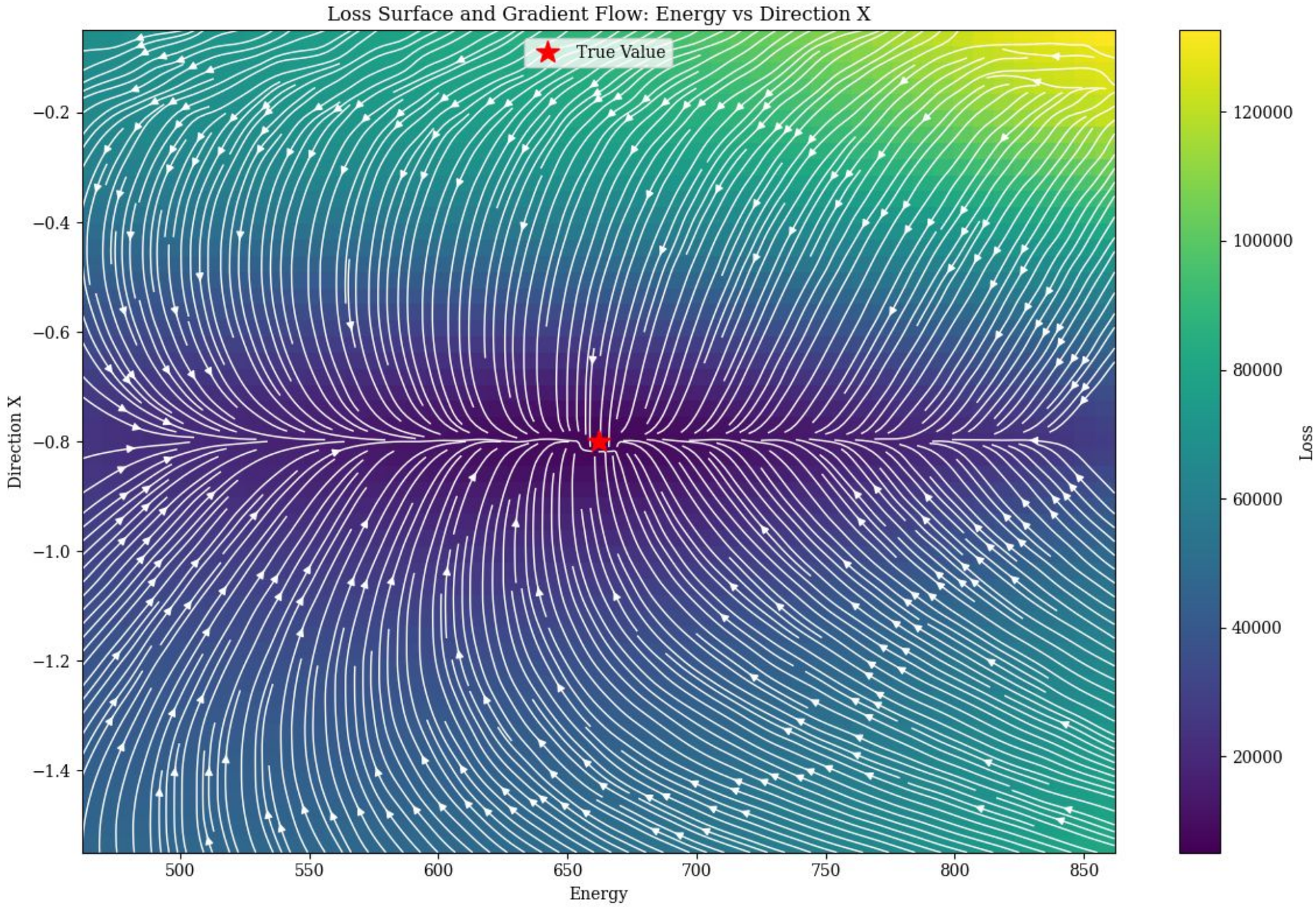
Energy/Direction



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Difference in Parameters True vs Simulation:

Energy: -4.14 MeV, Percent: -0.59 %

Position: 0.015, difference/pmt_radius: 0.379

Direction: 0.0032, Angular: 0.186 degrees

Event Parameters:

Energy: 700.90 MeV

Initial Position: (-0.46, -0.20, 0.55)

Initial Direction: (0.48, 0.20, -0.86)