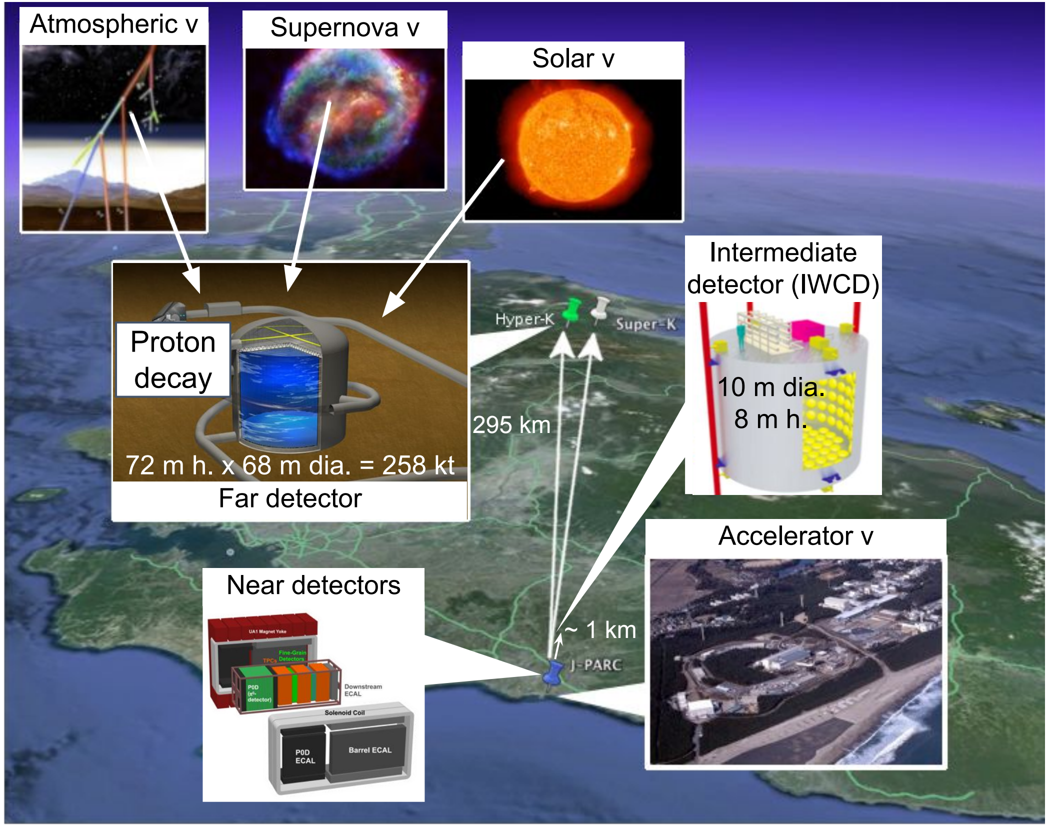
TRIUMF

Advances in simulation and reconstruction for Hyper-Kamiokande

Hyper-Kamiokande

Nick Prouse (TRIUMF)
ICHEP, 29th July 2020

The Hyper-Kamiokande experiment



Hyper-K builds on huge success of Super-K

Next generation neutrino experiment with two new water Cherenkov (WC) detectors

- 258 kt far detector @ 295 km
- 0.5 kt intermediate detector @ ~ 1 km

Broad & ambitious physics programme through comprehensive upgrades

- 8 x increase in fiducial mass
- Improved photo-detector technology
- Reduced systematics with new near & intermediate detector measurements

Improved analysis techniques required to realise Hyper-K's precision measurements

See **physics sensitivities** talks:
M. Scott, Wed 29 July, 18:45
T. Yano, Thu 30 July, 10:30

Hyper-K's WC detectors

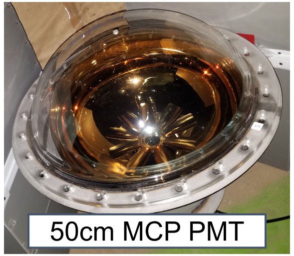
Hyper-K far detector

3rd generation of WC detectors at Kamioka

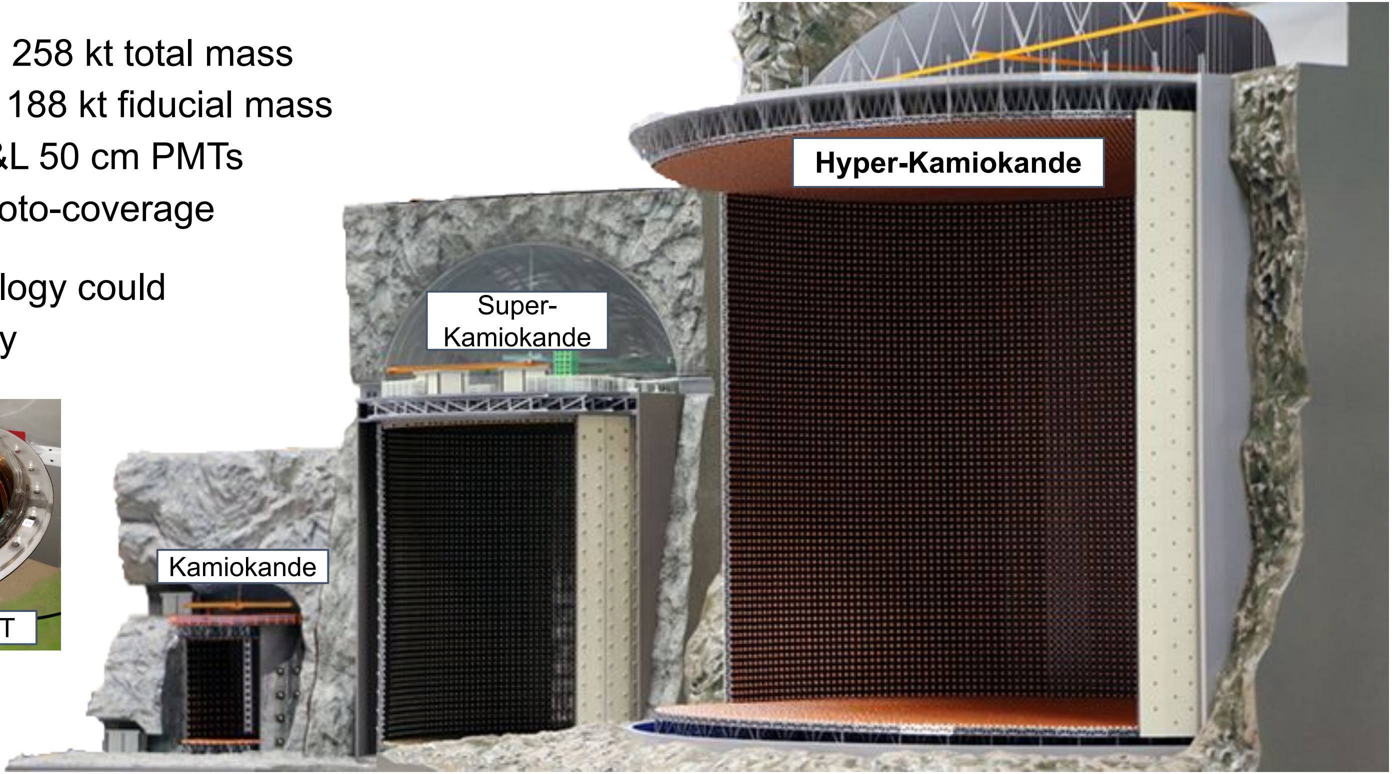
72 m tall x 68 m diameter = 258 kt total mass
188 kt fiducial mass

Baseline design: 40,000 B&L 50 cm PMTs
= 40% photo-coverage

New photo-detector technology could provide increased sensitivity

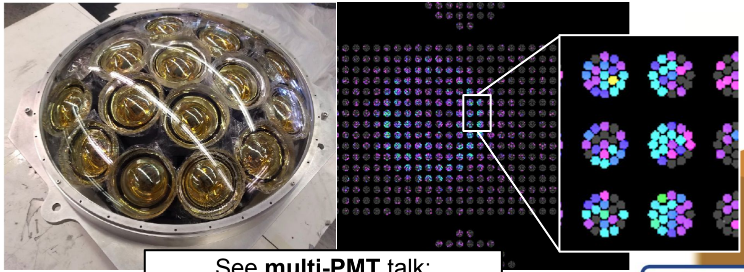


See **photo-detector** talk:
T. Tashiro, Fri July 31, 10:45



Hyper-K's WC detectors

Multi-PMT modules



See **multi-PMT** talk:
G. De Rosa, Fri July 31, 11:00

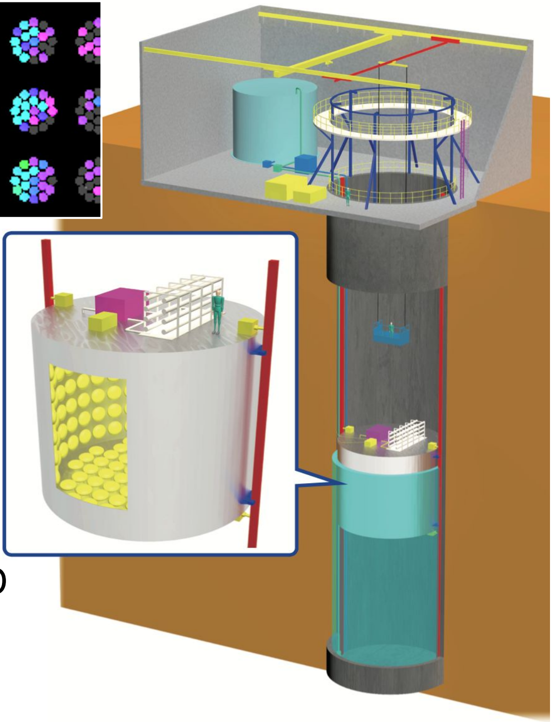
Necessary for small tank

8 cm PMTs: Better position resolution
< 1 ns timing resolution
Additional directionality information

Expect improvements in e.g. particle ID

Also under investigation:
Combining 50 cm PMTs + multi-PMT modules in far detector

See **HK near detectors** talk:
M. Hartz, Wed July 29, 19:00



Intermediate detector (IWCD)

Located ~ 1 km from beam source
8 m tall x 10 m diameter tank
~ 500 multi-PMT modules

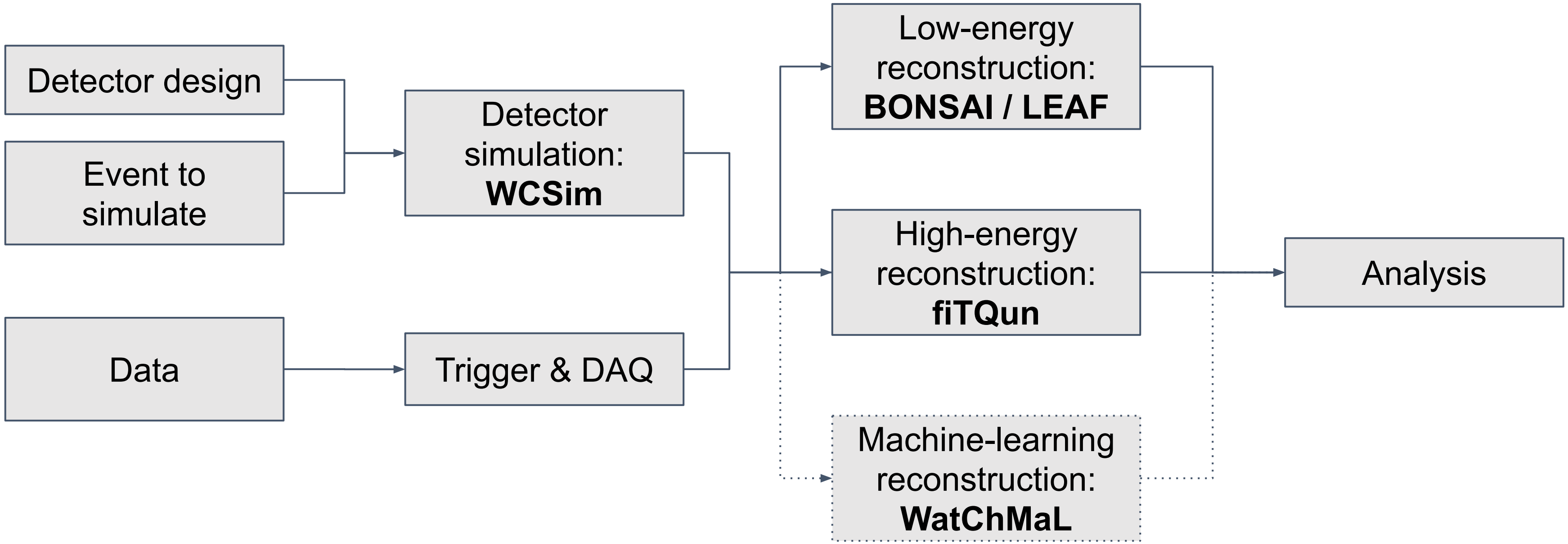
Measure flux + cross-section to reduce systematics at far detector

Measurements with high event rate, same technology and target nuclei as far detector

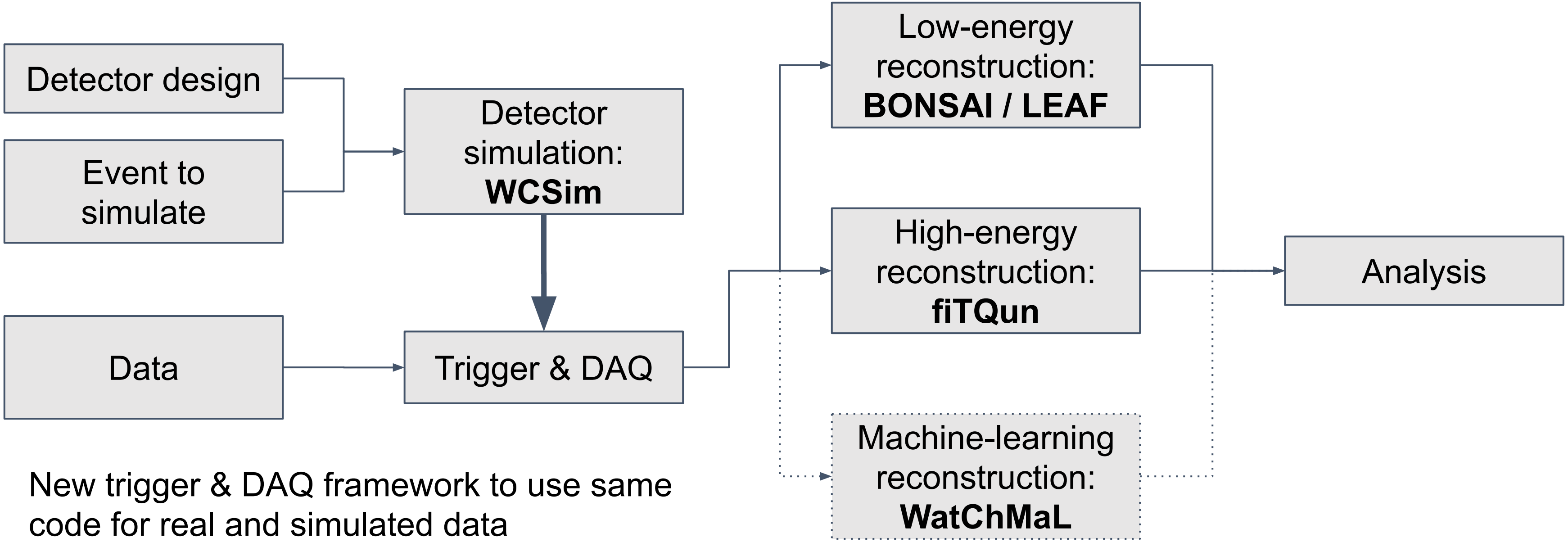
Moves vertically in ~50 m tall pit measuring different off-axis angles gives different ν energy spectra

New detector designs need improved simulation and reconstruction

Simulation & reconstruction overview



Simulation & reconstruction overview



New trigger & DAQ framework to use same code for real and simulated data

ToolDAQ: https://github.com/ToolDAQ

Simulation software

WCSim: Geant4-based WC detector simulation package

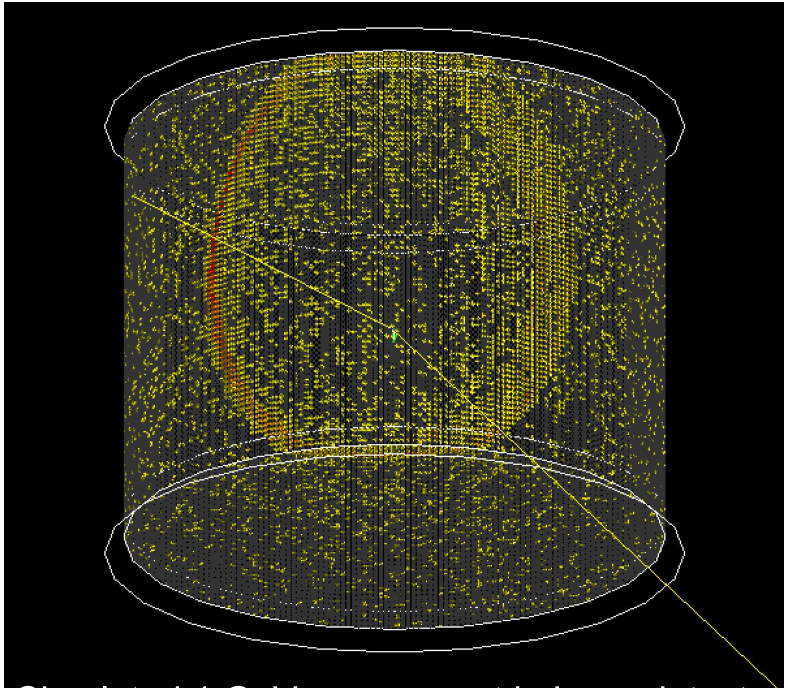
- Flexible simulation of water tank, PMTs and electronics
- Inputs:
  - Choice of detector geometry
    - Consistent simulation framework across detectors (HK & IWCD)
    - Well suited to detector optimisation studies
  - PMT & electronics specifications
  - Particles to simulate
    - Single particles / neutrino interaction products / background sources
- Output:
  - Digitized PMT hit times and charges
    - To feed in to reconstruction software
  - True particle track and PMT hit information
    - For debugging, investigating analysis, tuning reconstruction software

https://github.com/WCSim

Simulation software

See **HK OD** talk:
S. Zsoldos, Fri July 31, 11:45

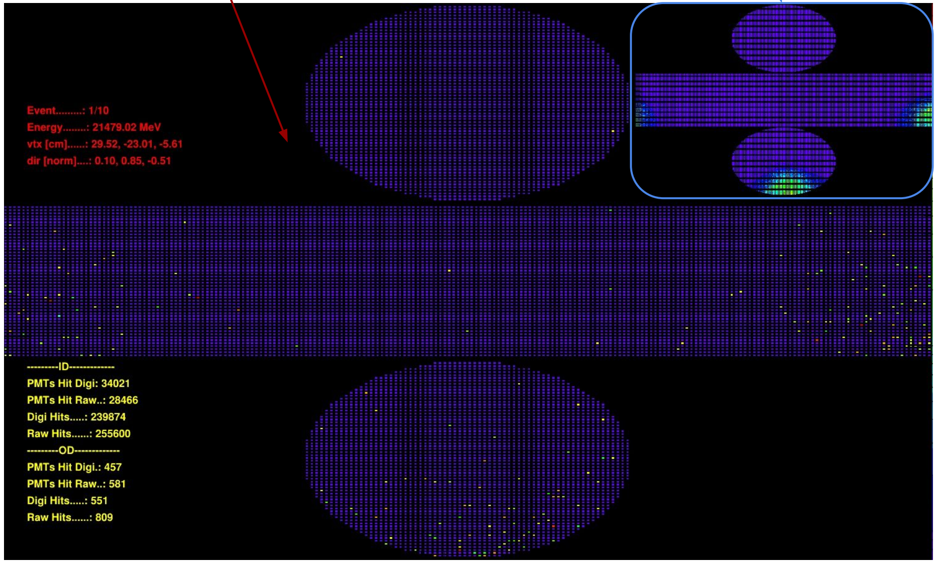
HK far detector (baseline design) simulation



Simulated 1 GeV muon event in inner detector

Inner detector (PMTs facing inwards)

Outer detector (PMTs facing outwards)

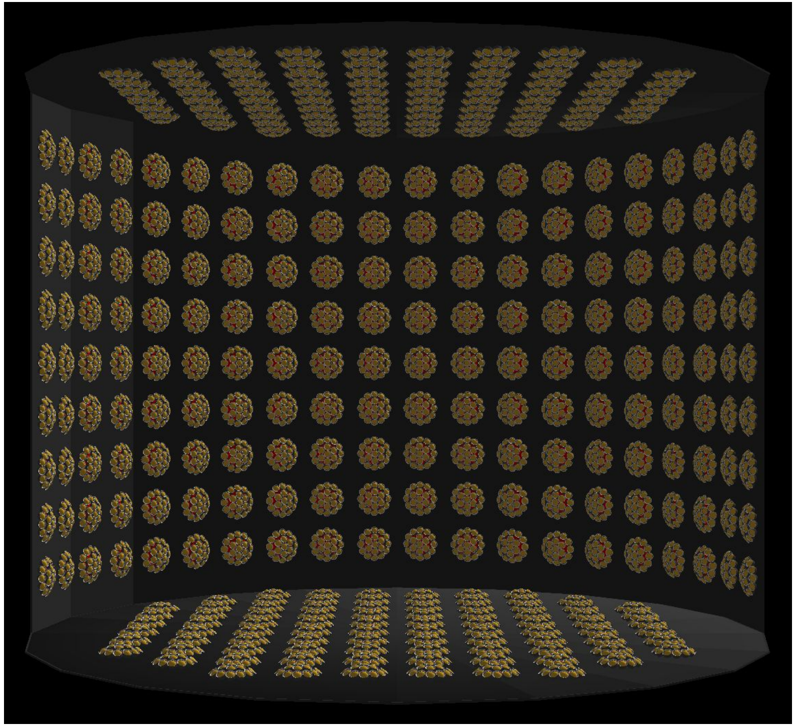


Simulated muon in outer detector

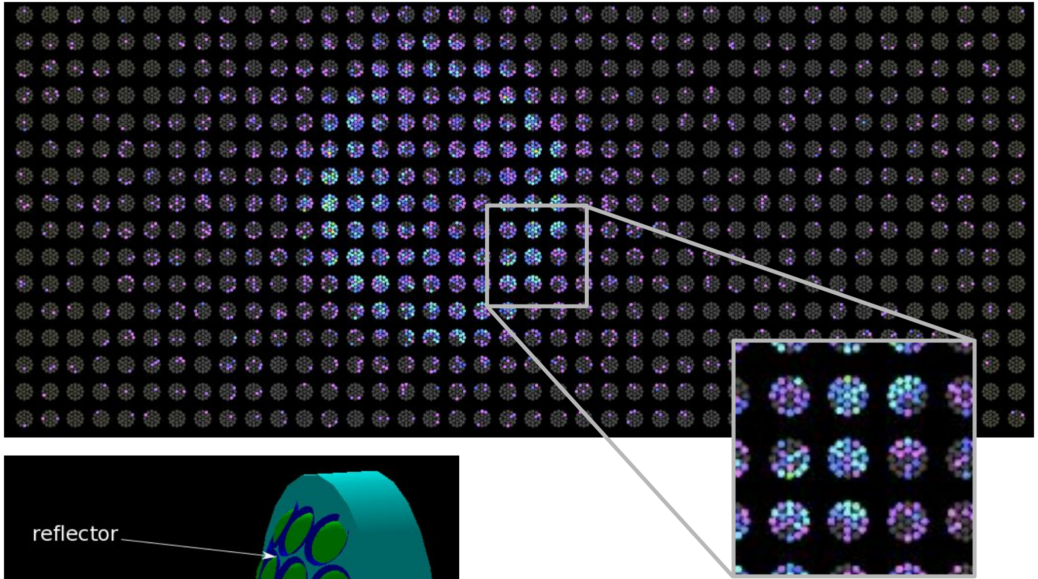
WCSim can easily simulate different detector setups

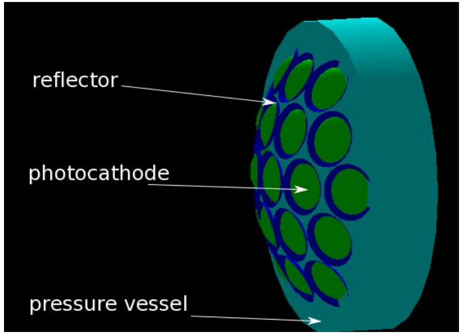
Simulation software

IWCD simulation (6 m tall inner detector)



IWCD simulation (10 m tall inner detector)





Full multi-PMT module geometry

WCSim can easily simulate different detector setups

Low-energy reconstruction software

BONSAI: Reconstruction for events with few MeV to 10s of MeV

- Position (vertex) reconstruction minimises goodness based on hit timing:

$$\underbrace{\boxed{g(\vec{v})}}_{\text{Goodness to maximise}} = \sum_{i=1}^{N} \underbrace{\boxed{w_i}}_{\text{Gaussian hit weights}} \exp\left(\left(-0.5\left(\left(\underbrace{\boxed{t_i}}_{\text{PMT hit times}} - |\underbrace{\boxed{\vec{x_i}}}_{\text{PMT locations}} - \underbrace{\boxed{\vec{v}}}_{\text{Candidate vertex}}|/c_{wat}\right)/\underbrace{\boxed{\sigma}}_{\text{Timing resolution}}\right)^2\right)\right)$$

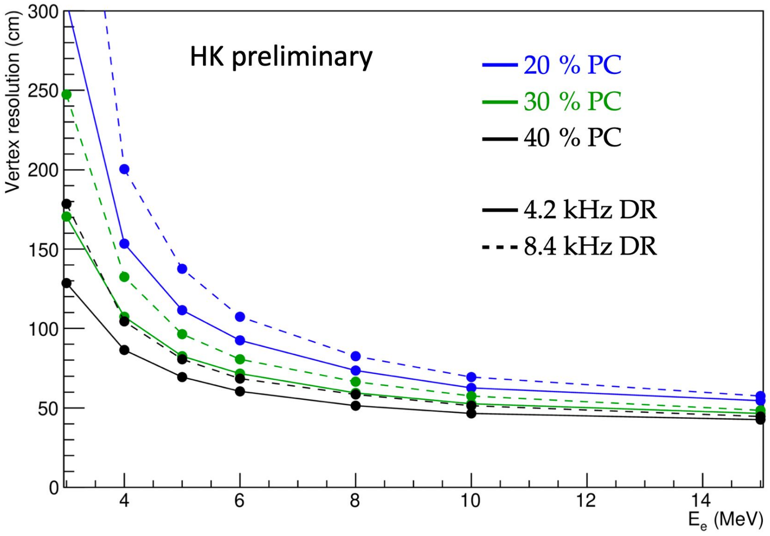
- Direction reconstruction uses circular KS test of hit pattern around the Cherenkov cone
- Energy reconstruction scales on number of hits observed around expected timing at each PMT

LEAF: More modern, flexible framework using same BONSAI algorithms

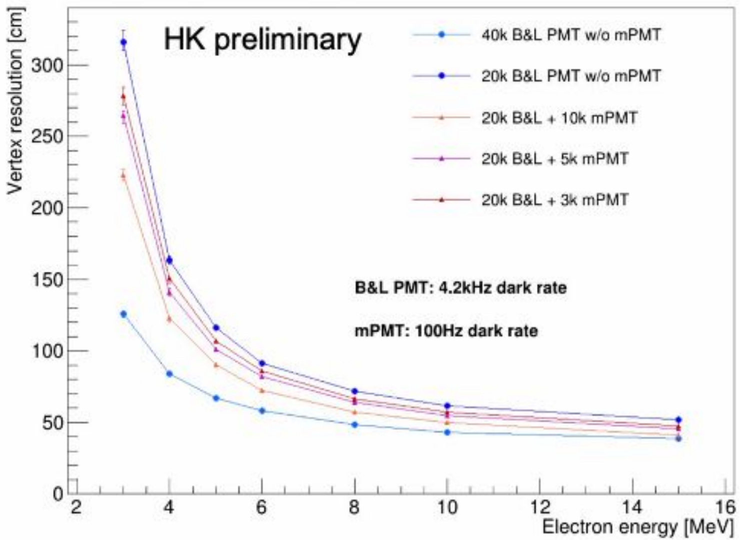
- New minimizer for vertex fitter
- Simpler to tune to different detector geometries

Low-energy reconstruction software

Testing different coverage and dark rate setups



Testing combinations of 50 cm PMTs and mPMTs



- Different detector designs can be tested to optimise for physics sensitivities
- Good resolutions as low as 3 - 5 MeV
- At low energies, total effective photo-coverage is most important factor
  - Low PMT dark rate also important to increase signal-to-noise ratio

High-energy reconstruction software

fiTQun: Advanced likelihood-based reconstruction for higher energies

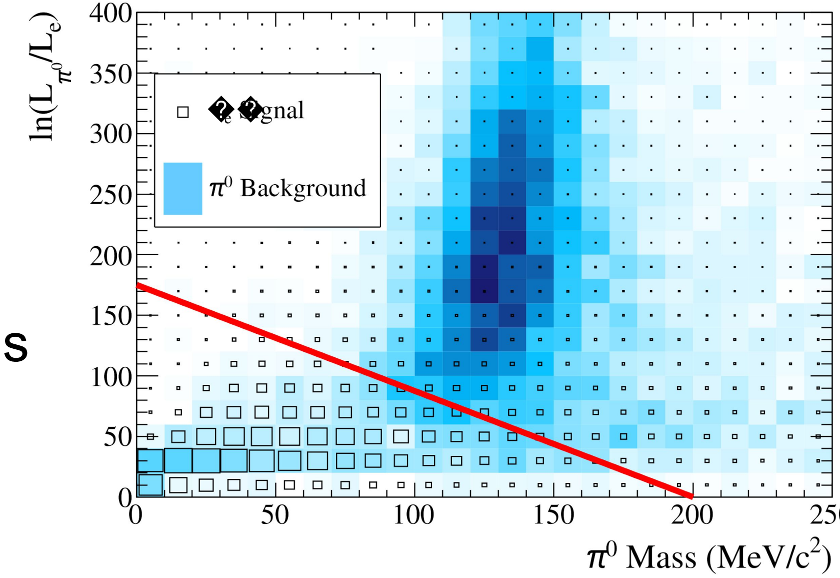
- Originally developed for Super-K detector
  - Based on algorithm of MiniBooNE: https://arxiv.org/abs/0902.2222
- Uses full information of unhit PMTs + time & charge of hit PMTs:

$$\underbrace{\boxed{L}}_{\substack{\text{Likelihood to}\\ \text{maximise}}}\left(\underbrace{\boxed{\mathbf{x}}}_{\substack{\text{Candidate event}\\ \text{hypothesis}}}\right) = \prod_{j}^{unhit} \underbrace{\boxed{P_j\left(unhit|\mathbf{x}\right)}}_{\substack{\text{Probability of}\\ \text{no hit at PMT}}} \prod_{i}^{hit} \underbrace{\boxed{P_i\left(hit|\mathbf{x}\right)}}_{\substack{\text{Probability of}\\ \text{hit at PMT}}} \underbrace{\boxed{f_q\left(q_i|\mathbf{x}\right)}}_{\substack{\text{Hit charge}\\ \text{probability density}}} \underbrace{\boxed{f_t\left(t_i|\mathbf{x}\right)}}_{\substack{\text{Hit time probability}\\ \text{density}}}$$

- Probabilities calculated based on direct + scattered + reflected light
- Likelihood ratios used to distinguish particle types and single-ring / multi-ring event topology hypotheses

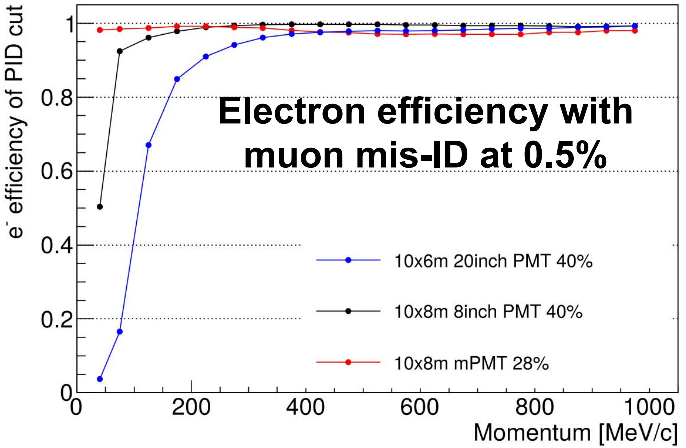
High-energy reconstruction software

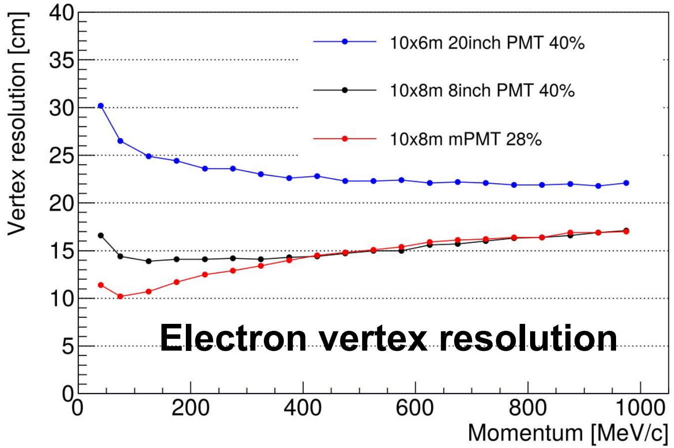
- π^0: significant background for ν_e signal
  - Decays to two gammas
    - Produces EM showers
  - When opening angle is small, looks like single electron ring
- fiTQun maximises likelihoods
  - Single-ring electron
  - 2-ring π^0
- Reconstruct mass for π^0 hypothesis
- 2D cut to reject background
  - Likelihood ratio
  - Reconstructed π^0 mass

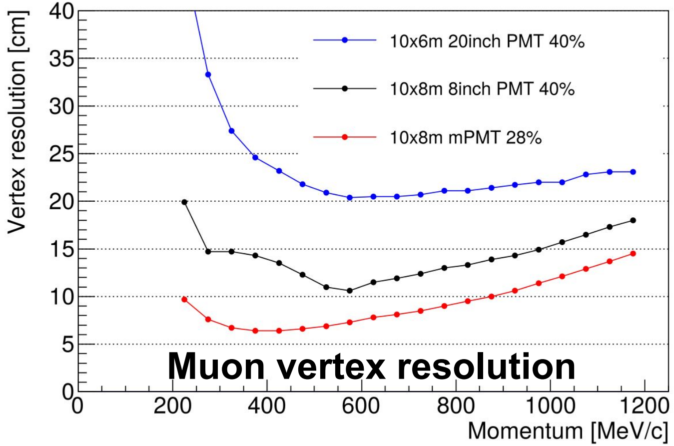


High-energy reconstruction software

fiTQun performance comparing different IWCD setups







- Good reconstruction resolutions & PID, down to ~ 50 MeV above energy threshold
- Improved timing & spatial resolution of mPMTs being utilised
  - Better performance even with lower photo-coverage

Machine learning reconstruction

Limit of traditional reconstruction methods is being reached

- Computation time is becoming a limiting factor
    - Larger detector with more PMTs
    - Improving resolutions requires more complex algorithms

Machine learning algorithms have potential to push further

- Potential to use all available information without detector model assumptions / approximations
- Very fast to run once neural networks have been trained
- Now becoming common throughout HEP applications
- But many new challenges...

Machine learning reconstruction

WatChMaL: cross-collaboration group formed to explore ML for WC

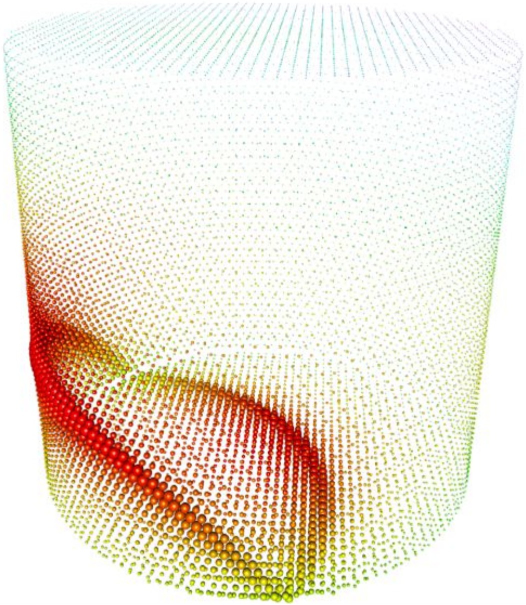
Common challenges for ML with WC detectors

- Cylindrical geometry
- High-resolution, sparse data

Many physics goals

- Maximise precision of new detectors
- Reconstruct complex event topologies
- Discriminate electron and gamma rings
- Improving detector calibration & systematics

WatChMaL.org

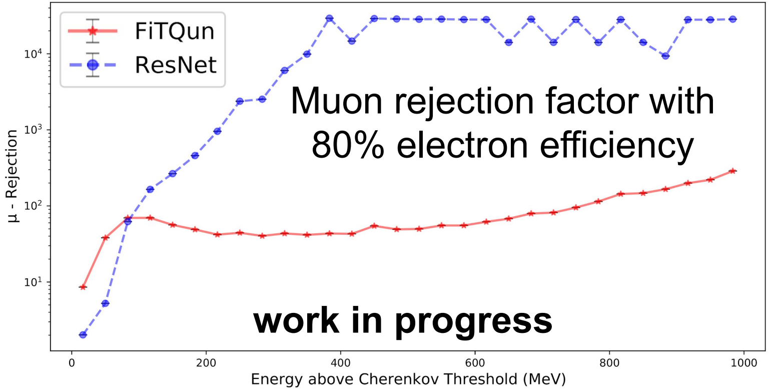


Machine learning reconstruction

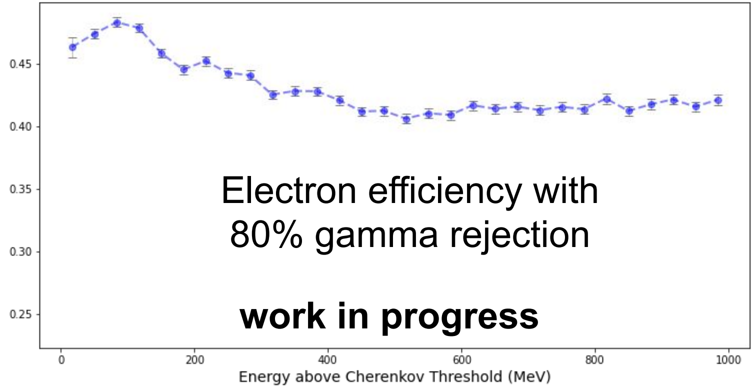
Initial studies of particle type classification in IWCD with ResNet CNN

ResNet-18 CNN architecture

- Cylinder unwrapped onto 40x40 pixel image
  - 1 mPMT per pixel
  - 38 channels: time, charge of the 19 PMTs per mPMT
- 3M of each of muons, electrons, gammas
  - Uniform positions throughout tank
  - Isotropic directions
  - Energies from 0 to 1 GeV above Cherenkov threshold



Significant improvement seen in muon vs electron discrimination



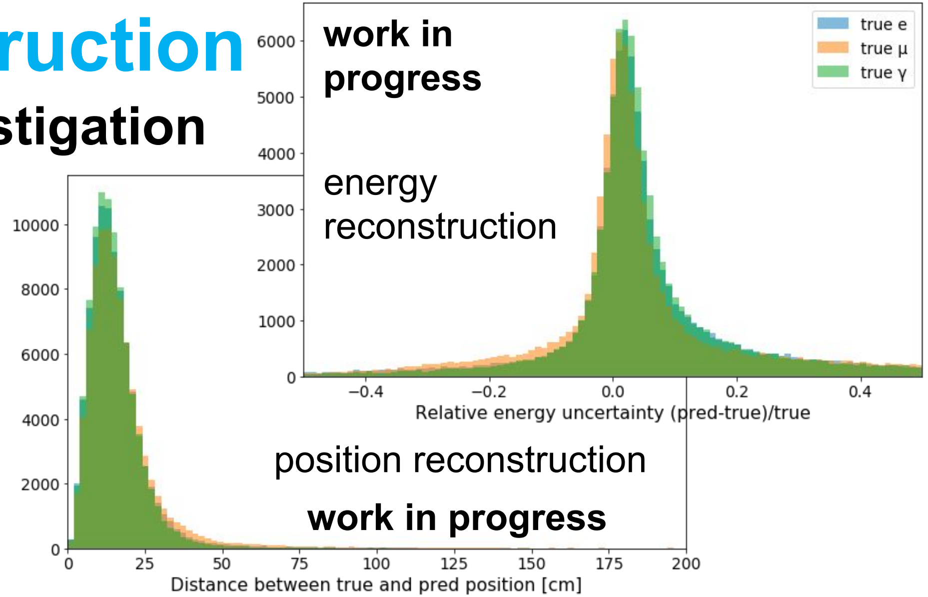
Neutral current gamma production is significant systematic uncertainty in oscillation analysis

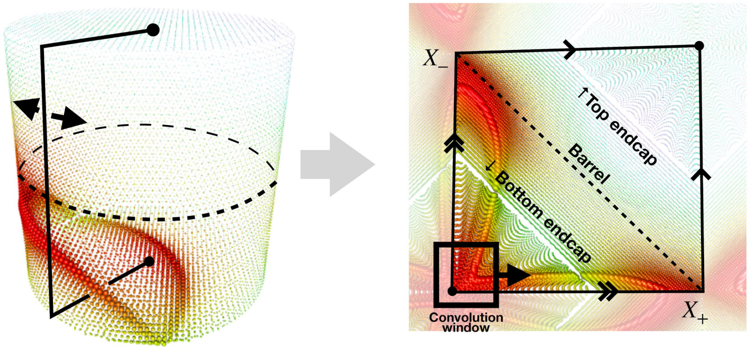
While no electron/gamma separation with fiTQun has been successfully used, ML looks promising

Machine learning reconstruction

Many other possibilities under investigation

- Reconstruction of physical quantities
- PointNet (point cloud NN) & Graph NNs for flexibility of detector geometries
- New methods for mapping cylinder to CNN images
- Generative networks to calculate fiTQun likelihoods
- Generative networks for improving simulation and detector systematics





Summary

Simulation and reconstruction framework has been developed for Hyper-Kamiokande's Water Cherenkov detectors

- Consistent simulation & reconstruction across detectors
- Simulation and reconstruction can adapt to different detector setups
- Enables detector design optimisation studies

Reconstruction packages give good reconstruction & PID performance

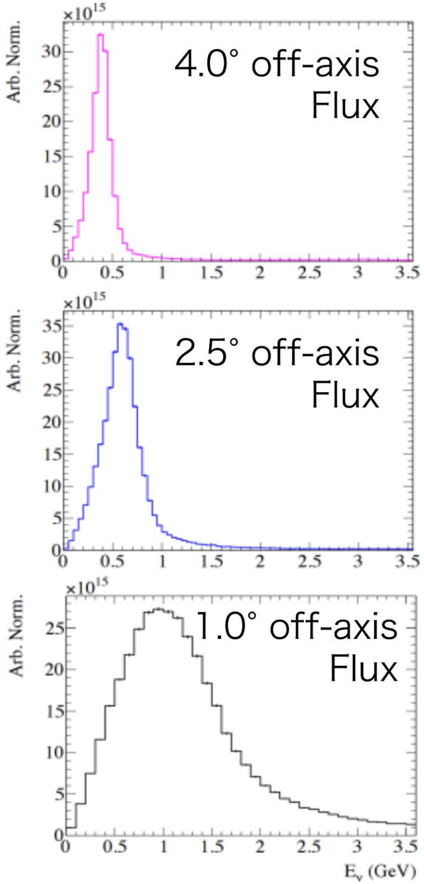
- Exploit improved photosensors of Hyper-K
- Smaller intermediate detector can use precision of mPMTs

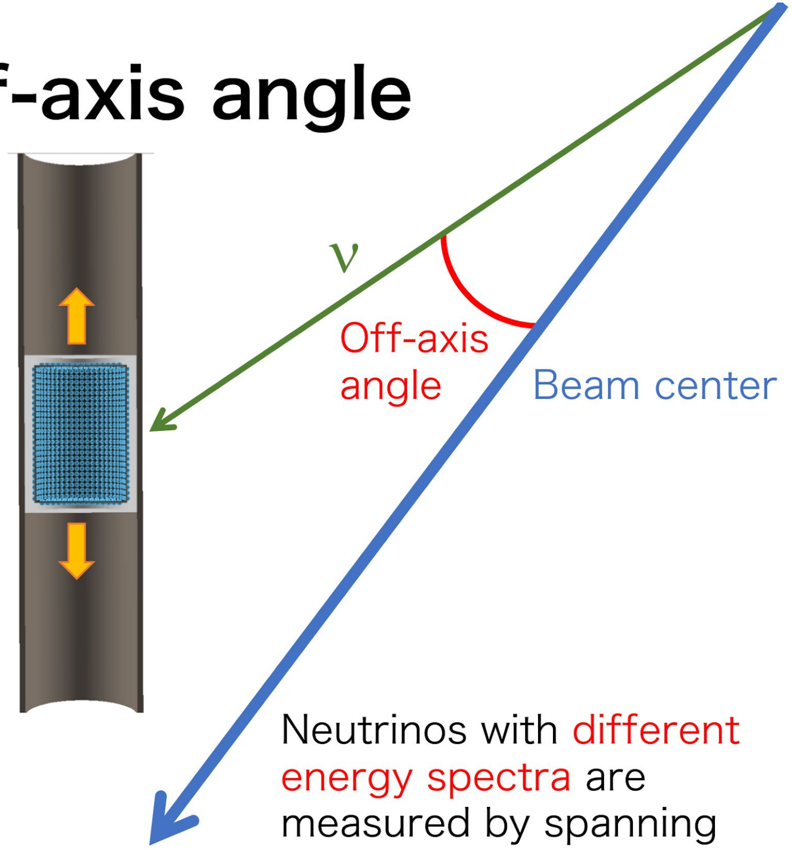
Machine learning can provide improved resolutions and new capabilities

- Electron vs muon PID suggests improvement from fiTQun
- Electron vs gamma statistical separation is possible
- Work underway on many new initiatives

Appendix

IWCD Spanning off-axis angle





Neutrinos with different energy spectra are measured by spanning off-axis angle

$$E_\nu = \frac{m_\pi^2 - m_\mu^2}{2E_\pi(1 - \beta_\pi \cos\theta)}$$

WCSim physics processing

- Kinematics of particles emitted by neutrino interaction or entering the detector are the input to WCSim.
- Physics processes of particles after the neutrino interaction are simulated by Geant4.
  - Particle track in water, interaction with nuclei, and Cherenkov radiation
- Geant4 also tracks Cherenkov photons.
- Many parameters describing material properties are taken from Super-K calibration and simulation
  - Water, black sheet, glass

PMT description in WCSim

When a photon reaches PMT surface, output signal is simulated according to PMT properties.

- PMTs are described by some functions and parameters
    - Overall efficiency for a photon to register a charge, including the quantum efficiency and collection efficiency
    - Single photo-electron distribution
    - Timing response function
    - Dark noise rate
- Users can modify PMT properties easily

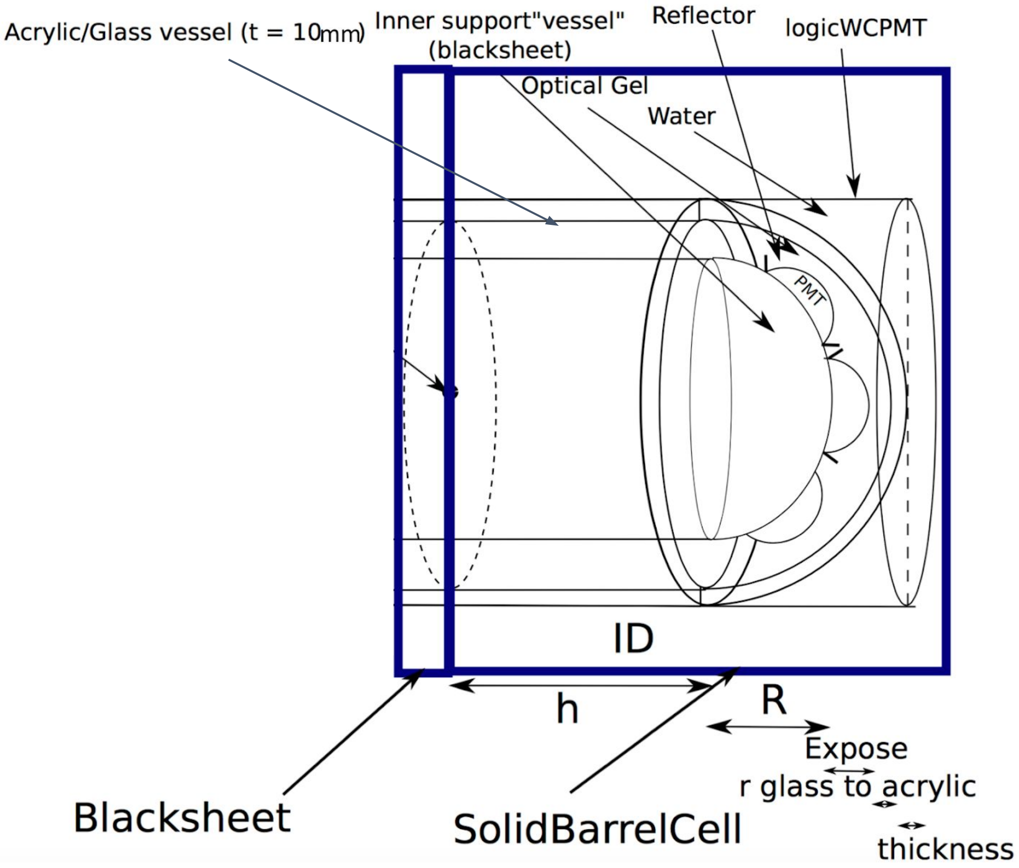
Electronics in WCSim

- As dark noise, add random 1 photo-electron hit to each PMT at a given rate
- Convert hits by real photon and dark noise, and then digitize the hits
  - PMT-by-PMT threshold is applied
  - Timing and charge smearing can be applied
- Issue triggers by using number of digitized hits in a given sliding timing window

WCSim: mPMT implementation

- Acrylic vessel
- Optical gel
- Aluminum reflector
- 3inch PMT
- Inner support structure

OD simulation is under construction

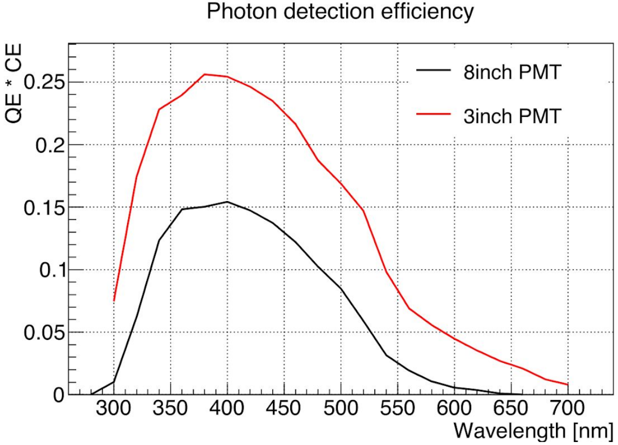


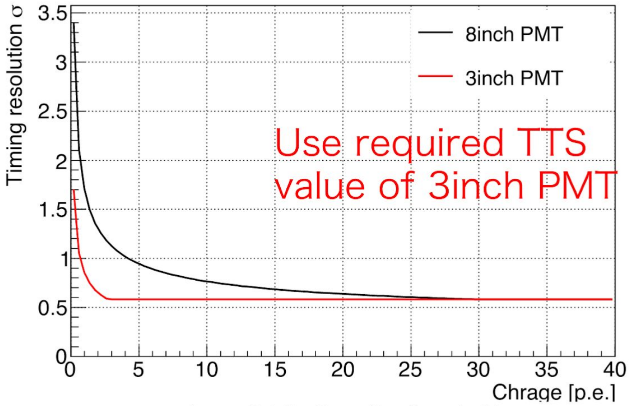
WCSim: Implemented mPMT properties

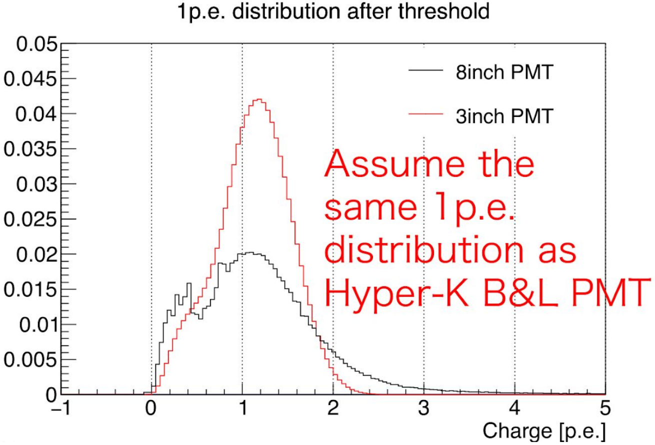
New measurements of PMT properties are underway

8inch PMT properties based on old LBNE measurements

QE is taken from KM3NeT measurement
doi: 10.1063/1.4902786







fiTQun direct light charge prediction

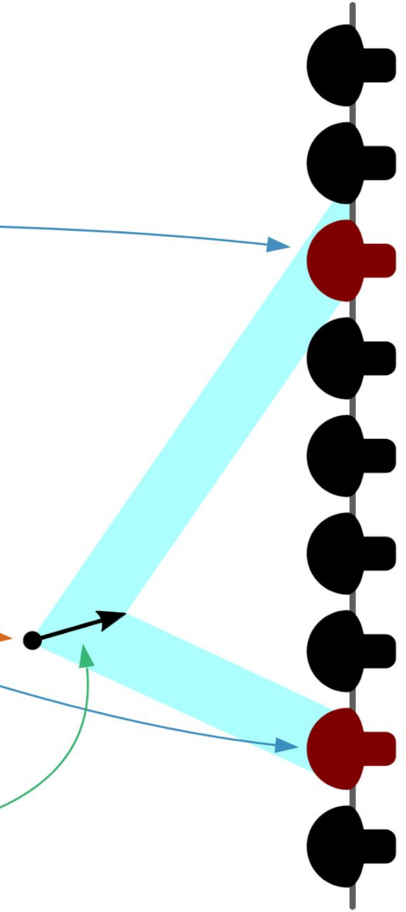
C. Vilela, SBU

$$\boxed{\mu^{dir}} = \boxed{\Phi(p)} \boxed{\int ds} \, g(p, s, cos\theta) \; \Omega(R) \; T(R) \; \epsilon(\eta)$$

The direct light charge prediction μ is evaluated at each of the hit photosensors

The overall amount of light is governed by the function Φ, which depends on particle type and momentum

The factors g, Ω, T and ϵ are evaluated in an integral which is computed over the length of the track s

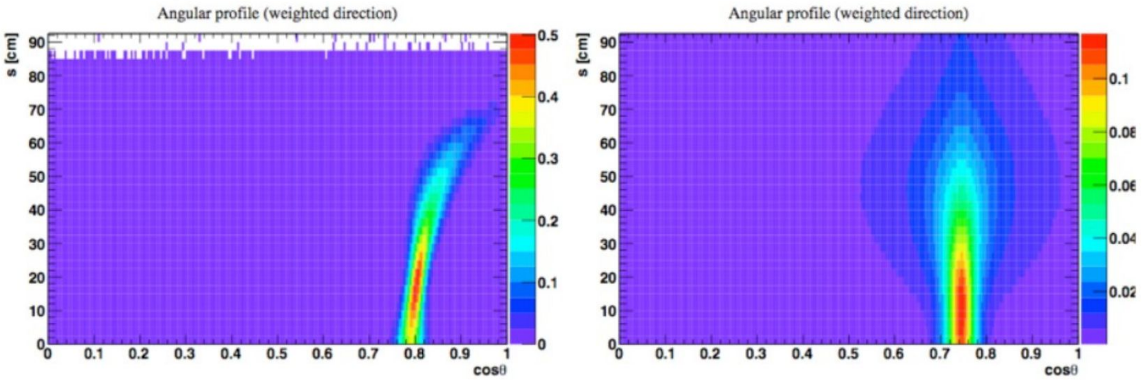


C. Vilela, SBU

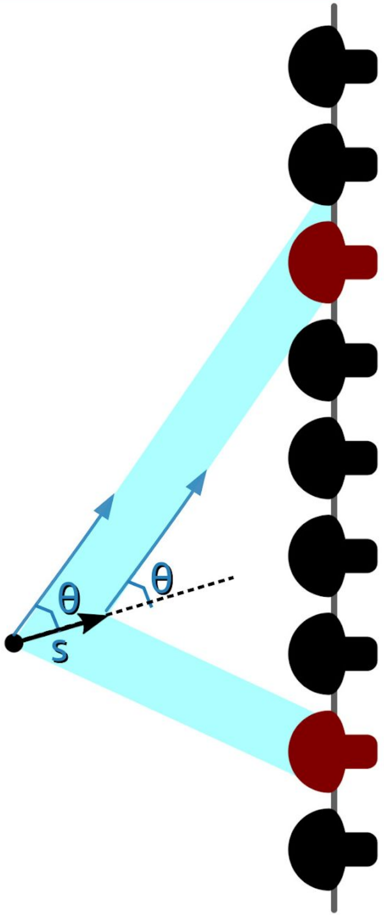
fiTQun direct light charge prediction

$$\mu^{dir} = \Phi(p) \int ds \, \boxed{g(p, s, cos\theta)} \, \Omega(R) \, T(R) \, \epsilon(\eta)$$

The function g encodes the Cherenkov emission profile



Muon (left) and electron (right) emission profiles at 300 MeV/c



- Cone collapse differs for particles of different mass
- This is all the information used for individual ring PID

fiTQun direct light charge prediction

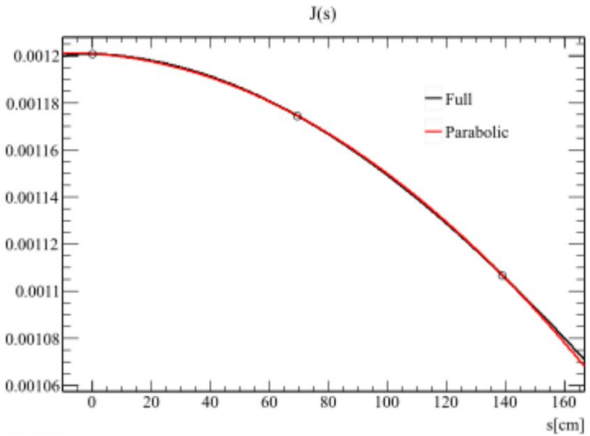
C. Vilela, SBU

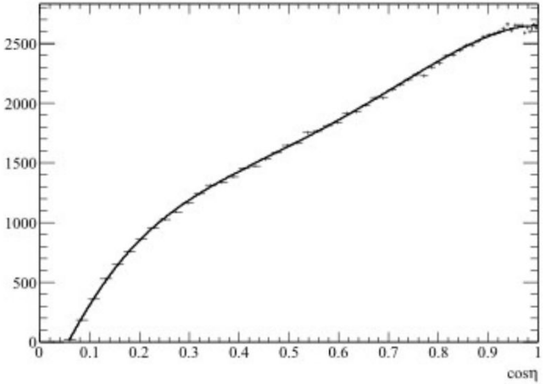
$$\mu^{dir} = \Phi(p) \int ds\, g(p, s, cos\theta) \boxed{\Omega(R)} \boxed{T(R)} \boxed{\epsilon(\eta)}$$

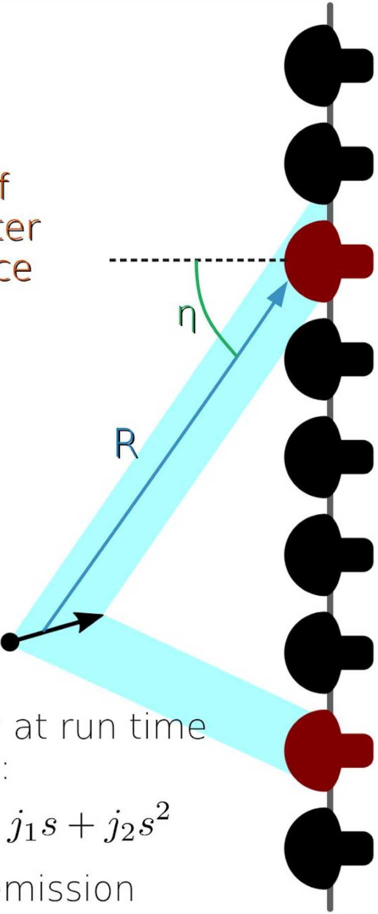
Ω reflects the change in apparent scale of the photosensor as a function of distance

T gives the amount of light attenuation in water as a function of distance

ϵ represents the angular response of the photsensor accounting for effects such as the shadowing due to adjacent PMTs and the shape of the photocathode







The integral is not computed explicitly at run time

- A parabolic approximation is used:

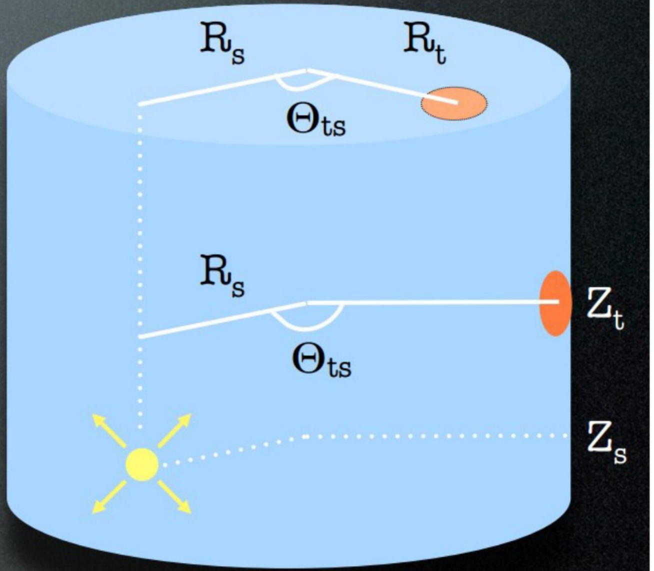
$$J(s) = \Omega(R)\, T(R)\, \epsilon(\eta) \approx j_0 + j_1 s + j_2 s^2$$

- The integral over the Cherenkov emission profile is tabulated

C. Vilela, SBU

fiTQun indirect light charge prediction

- Currently assume a **cylindrical geometry**
- Tabulate $\dfrac{d\mu^{indirect}}{d\mu^{direct,iso}}$ $(= A_{scat})$
  - Source direction (θ_s, ϕ_s)
  - Source position (Θ_{ts}, R_s, Z_s)
  - Z_t for PMTs on the sides
    - $A_{side}(\theta_s, \phi_s, \Theta_{ts}, R_s, Z_s, Z_t)$
  - R_t for PMTs on the ends
    - $A_{end}(\theta_s, \phi_s, \Theta_{ts}, R_s, Z_s, R_t)$



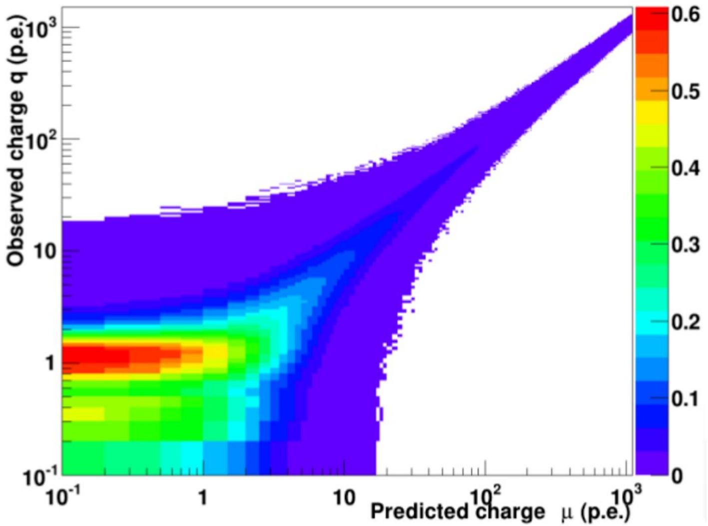
fiTQun PMT response

C. Vilela, SBU

Charge

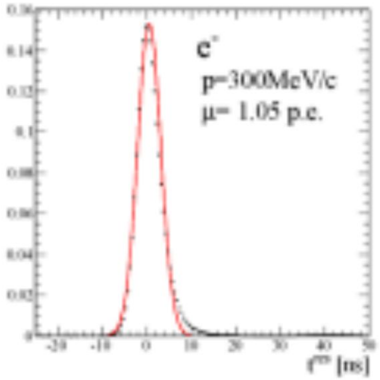
- PDFs of the observed charge for a given true mean obtained from Monte Carlo simulation
- Hit probability functions are extracted from these distributions

Charge PDF f(q|μ)

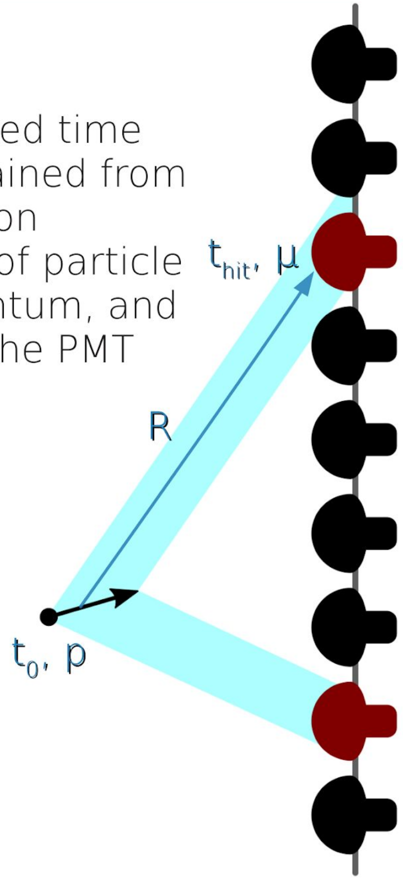


Time

- Time-of-flight corrected time distributions are obtained from Monte Carlo simulation
- Stored as a function of particle type, particle momentum, and predicted charge at the PMT



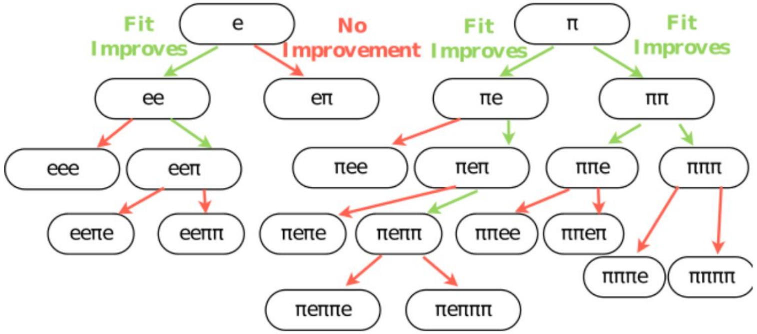
$$t_{corr} = t_0 - \left(t_{hit} - \frac{Rn}{c} - \frac{s}{2c}\right)$$

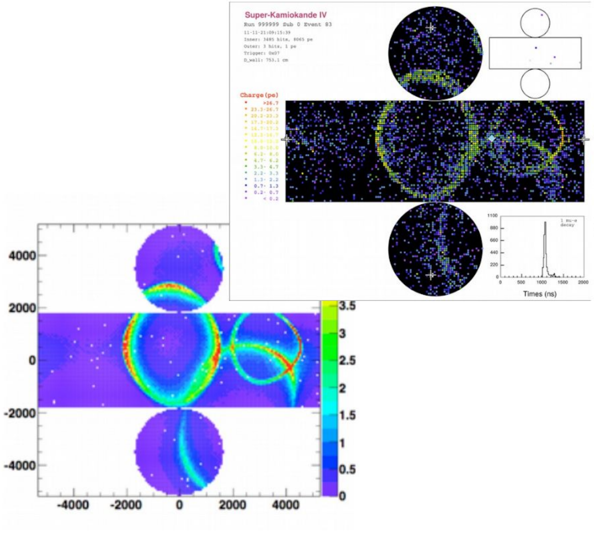


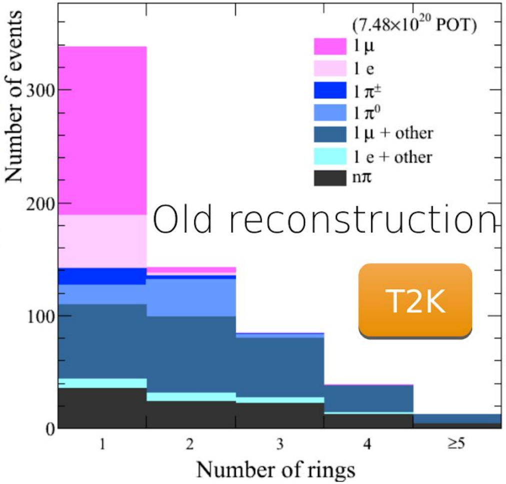
C. Vilela, SBU

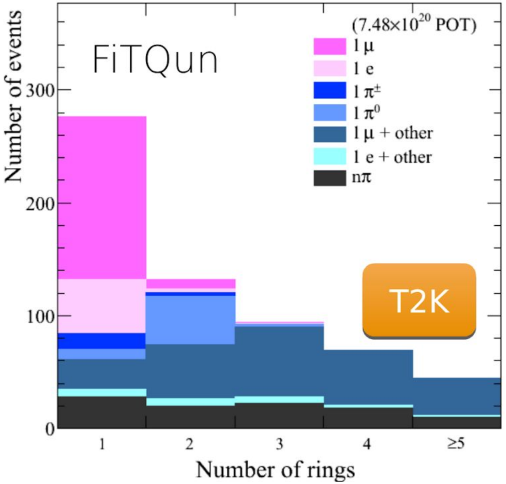
fiTQun multi-ring fitter

- Start from single-ring fits and sequentially add e-like or π-like ring until no improvement is seen.
- Once best-fit hypothesis is found, improve by fitting additional particle hypotheses (e.g., μ-like)

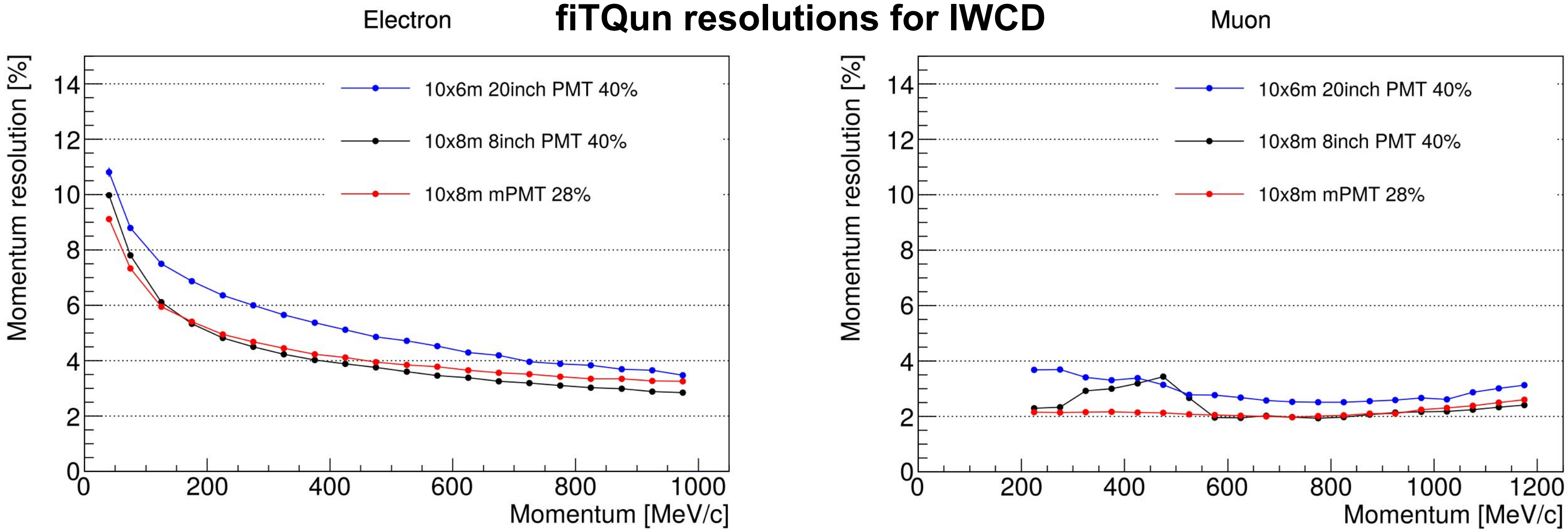








fiTQun momentum resolution

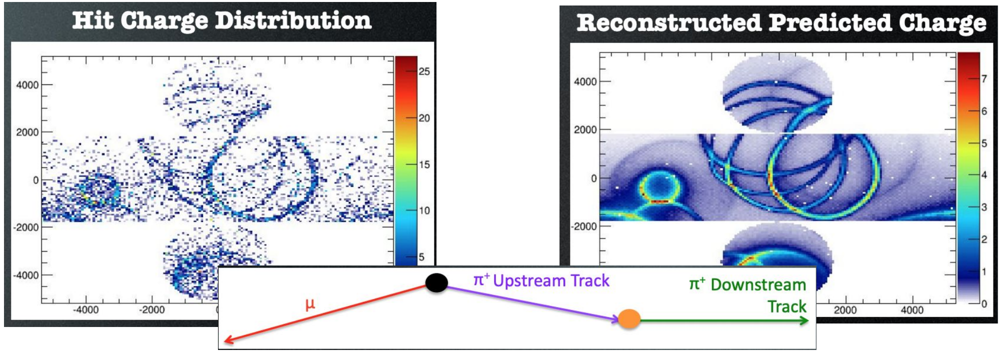


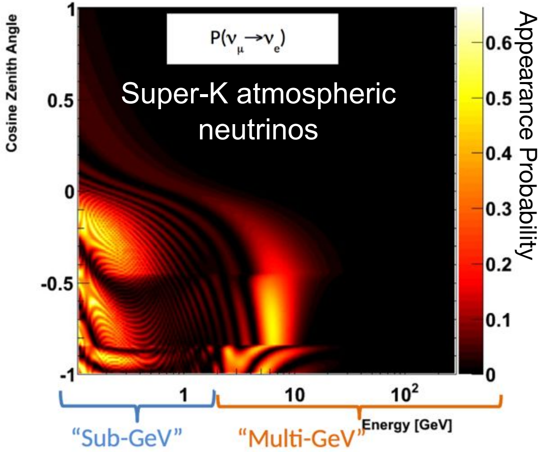
- Good resolution down to ~50 MeV above threshold
- Improved timing & spatial resolution of mPMTs being utilised
    - Better resolutions even with lower photo-coverage

ML Physics goals

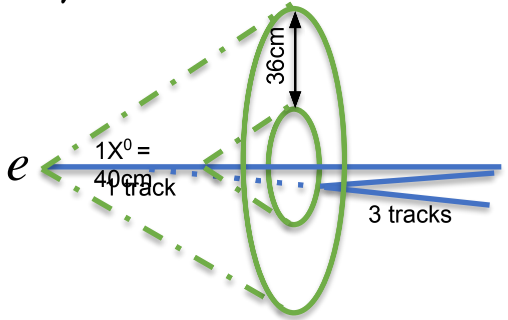
TRIUMF

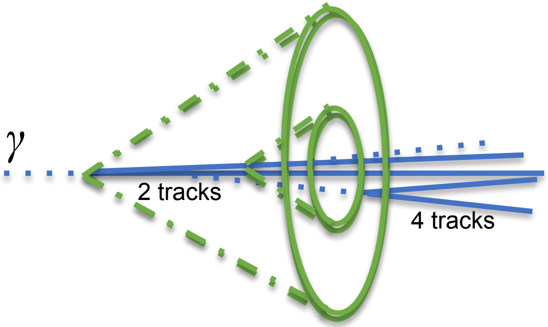
Complex event topologies: multi-GeV events

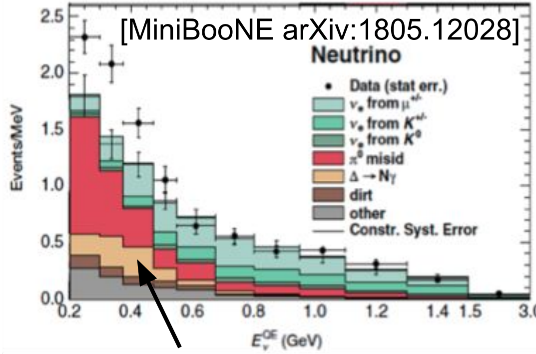




e^- / γ discrimination & improved π^0 identification



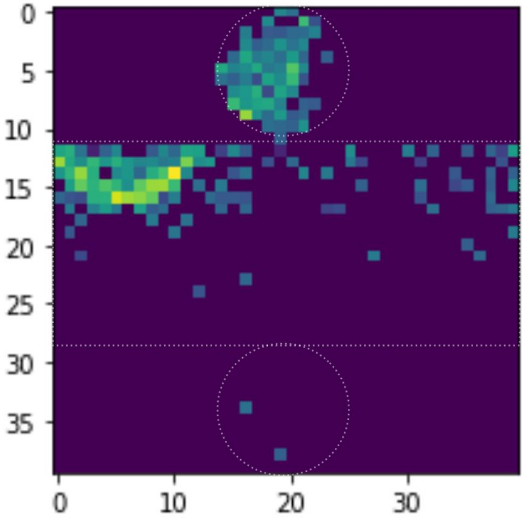




High uncertainty on NCγ background

Machine learning dataset

- For most studies in this talk:
  - e/μ/γ events (3M events each)
  - IWCD with mPMTs
  - flat distribution in $E\text{–}E_{\text{Cherenkov-thr.}} = 0 \sim 1000$ MeV
  - uniformly distributed in full tank (no veto for partially-contained tracks)
  - 4π direction



- For each PMT charge and time (though sometimes only charge is used)

- Individual PMTs belonging to the same mPMT module are all placed at the same pixel. Since each mPMT has 19 small PMTs, there are 19 input layers like the one shown.

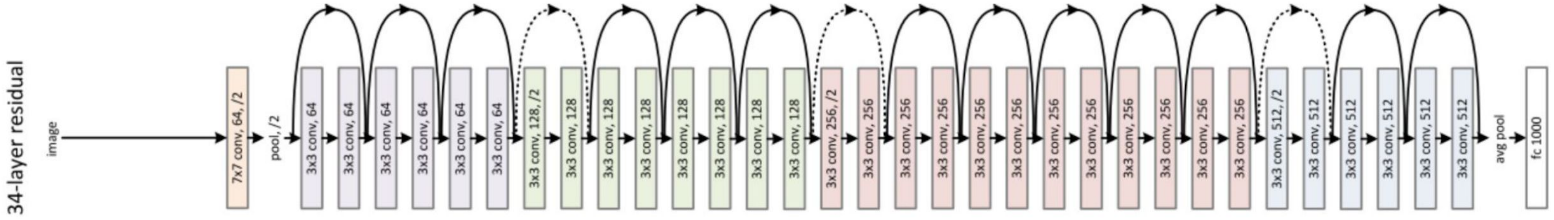
- IO is sped up by only loading hit information from disk, and populating tensor at runtime

CNN architecture

- From earlier studies ResNet* seems to work well.
  * K. He et al., arXiv:1512.03385
- In general deeper is better, but for practical purposes using 18 layers.
- Later will also discuss other networks like PointNet.

Results from earlier studies with *easier* dataset:
(side-going events from vertex fixed to center of tank, barrel only)

Model	γ Rejection at 50% e signal efficiency	AUC
LeNet-9 CNN	85.5 (7.01)	0.780
ResNet-50 CNN	90.4 (10.55)	0.836
ResNet-101 CNN	90.3 (10.46)	0.836
ResNet-152 CNN	**90.7 (11.04)**	**0.841**
DenseNet-121 CNN	89.7 (9.75)	0.823



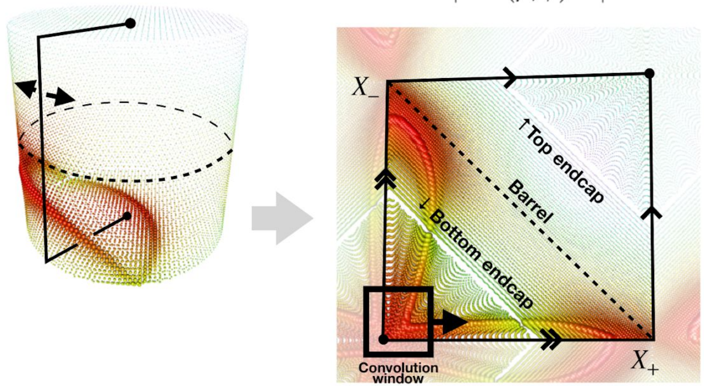
Topological map to square

Cut open along solid line and map to square, with $W(\rho, z)$ chosen to preserve area:

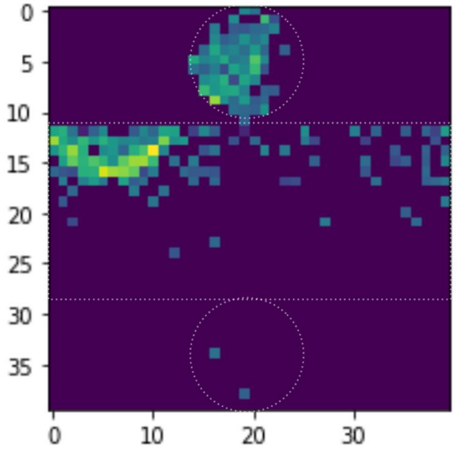
$$X_{\pm} = W(\rho, z)\frac{\pi \pm \phi}{2\pi} \qquad W(\rho, z) = \sqrt{\frac{\rho^2 + 2Rz + RH}{R^2 + RH}}$$

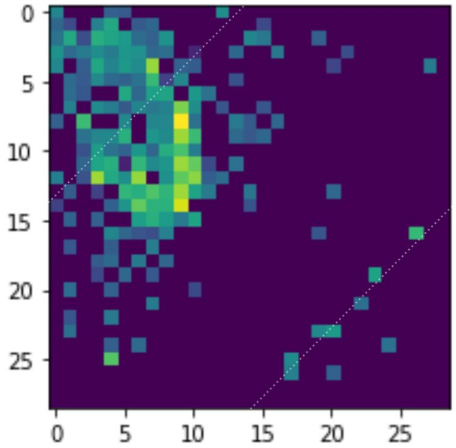
Solve differential eq. for constant Jacobian

$$\mathrm{d}X_+\,\mathrm{d}X_- = \left|\frac{\partial(X_+, X_-)}{\partial(\rho, \phi)}\right| \mathrm{d}\rho\,\mathrm{d}\phi$$

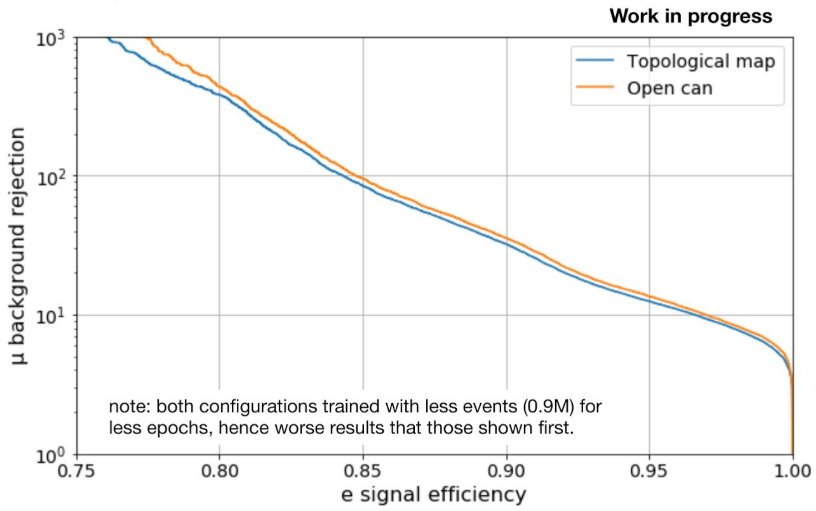


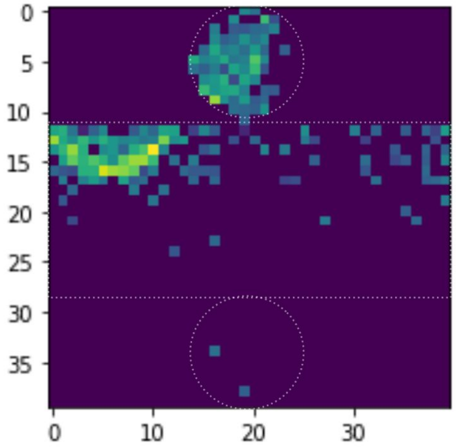
The PMTs are then put on a square grid which can be fed to machine learning libraries. Prior to convolution, pad sides according to **identification given by arrows** to embody topology of 2-sphere.

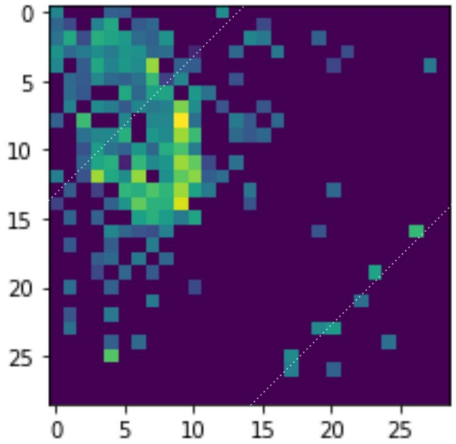




Topological map to square







Interestingly, the original rep (open can) seems to work better

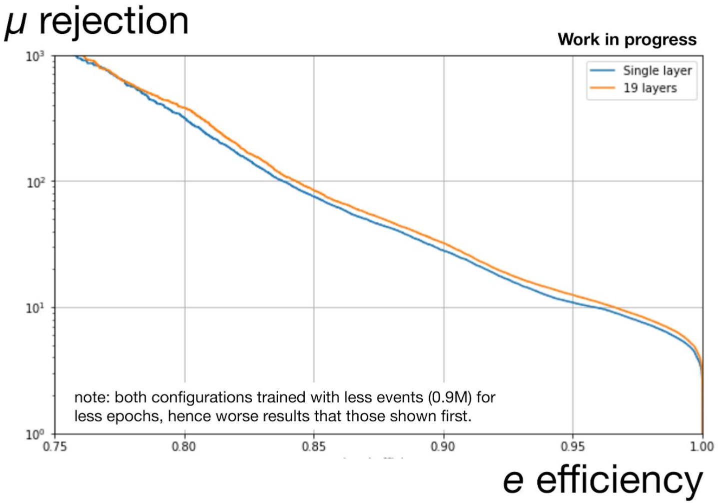
but difference is small

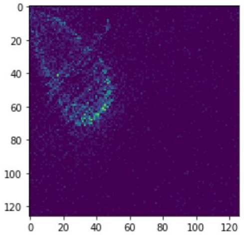
→ maybe because of explicit
ϕ-symmetry for barrel?
PID is mostly due to local features?

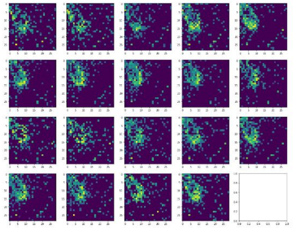
note: Using separate networks for top/ bottom/barrel gives much worse results

Representation of mPMTs

- **Single layer**
  Give each 3" PMT a pixel, and put on a single layer
- **19 layers**
  Put whole mPMT module onto a pixel, and put each 3" PMT on its own layer (19 3" PMT / mPMT → 19 layers for each ch)



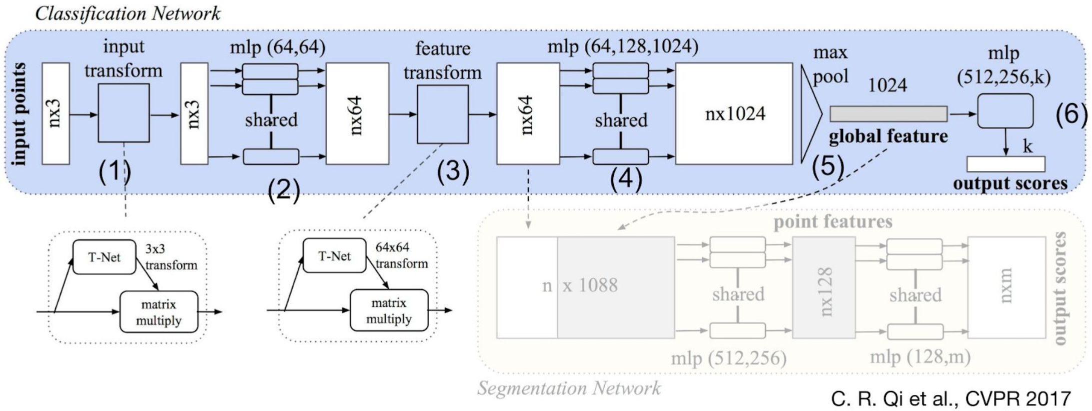




19 layers *slightly* better?
Reasonable since with single layer network doesn't know which pixel is looking in which direction. However close to order of random fluctuations.

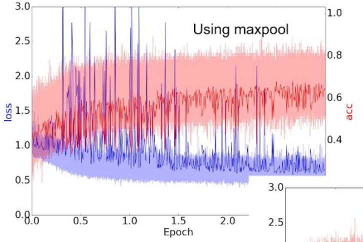
Also PMT light yield can vary by position in module, maybe network can pick this up better.

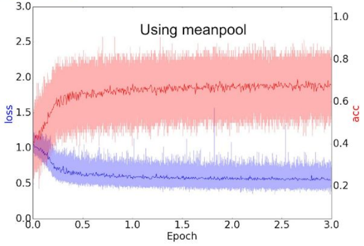
PointNet for e/μ/γ



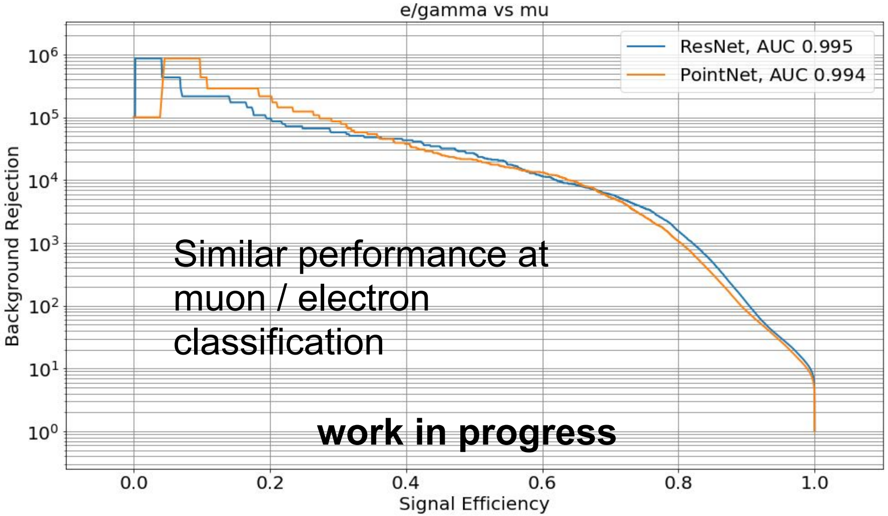
C. R. Qi et al., CVPR 2017

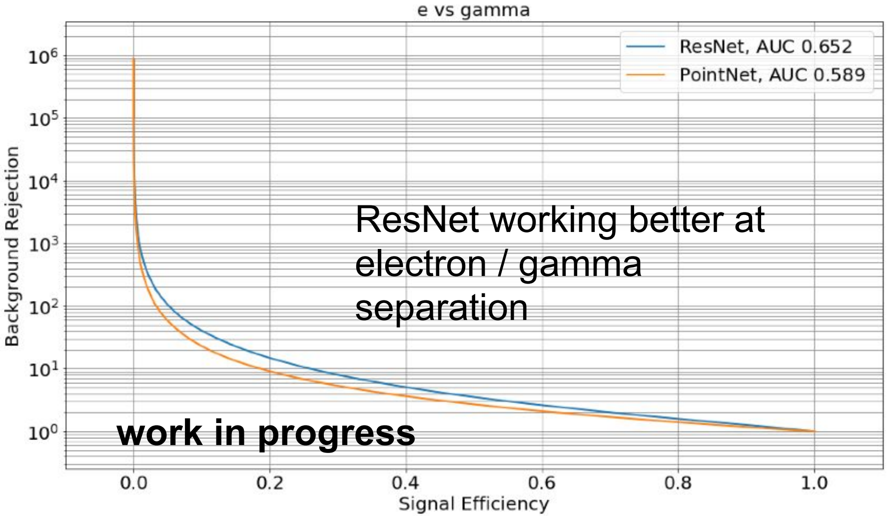
- Each PMT hit represented as a point (charge+time+pos)
- Network learns linear transformation to rotate input and feature vectors, then applies symmetric pooling operation
- We notice mean pooling gives better results than max pooling in original paper
  → consistent with experience from traditional reconstruction that all PMT hit info contribute





Exploring PointNet (point cloud neural network) for greater flexibility with detector geometries





PointNet uses less ‘local’ features

- May work better at low-E (hits distributed more sparsely)
- May work better at regression tasks (position, energy, direction)

Position/energy reconstruction

- Same network as for PID classification, but interpret network output as:
    1. E_{pred}
    2. $\log \sigma_E^2$
       pred. energy resolution
    3. x_{pred}
    4. y_{pred}
    5. z_{pred}
    6. $\log \sigma_{\text{pos}}^2$
       pred. position resolution

- To give the network geometry information, PMT positions and directions are passed in as additional input layers

Loss defined as

$$L = L_E + L_{\text{pos}}$$

$$L_E = \frac{(E_{\text{pred}} - E_{\text{true}})^2}{2\sigma_E^2} + \frac{1}{2}\log \sigma_E^2$$

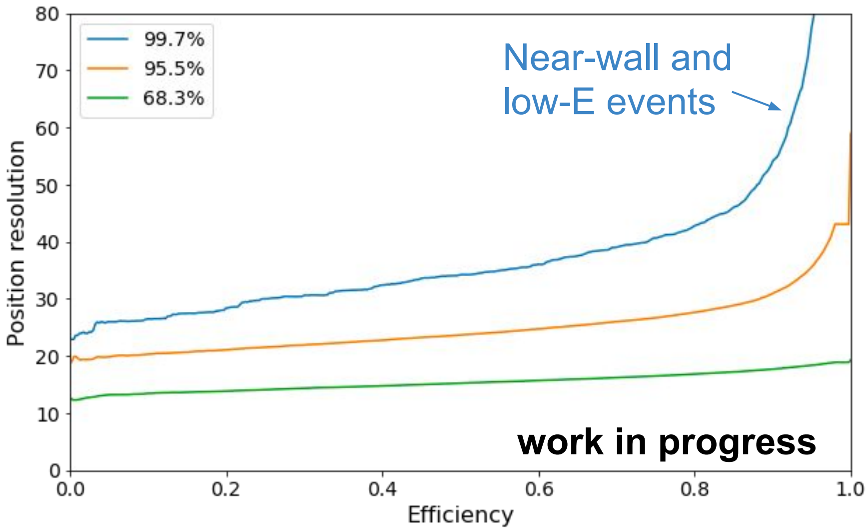
$$L_{\text{pos}} = \frac{(\mathbf{x}_{\text{pred}} - \mathbf{x}_{\text{true}})^2}{2\sigma_{\text{pos}}^2} + \frac{3}{2}\log \sigma_{\text{pos}}^2$$

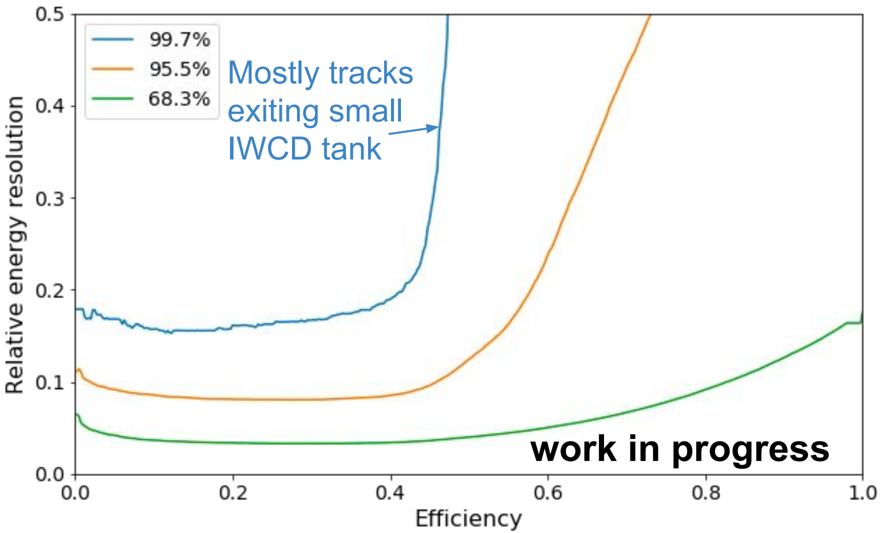
introducing $\log \sigma^2$ has couple of benefits:

1. adjust relative scaling of L_E and L_{pos}
   similar technique used in A. Kendall et al., CVPR 2018
2. remove bias due to events that are inherently impossible to reconstruct
   e.g. energy for uncontained events
3. can select well reconstructed events

Machine learning reconstruction

Position and energy reconstruction using ResNet

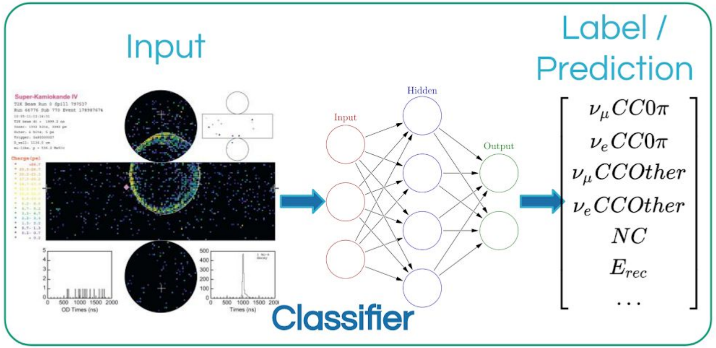


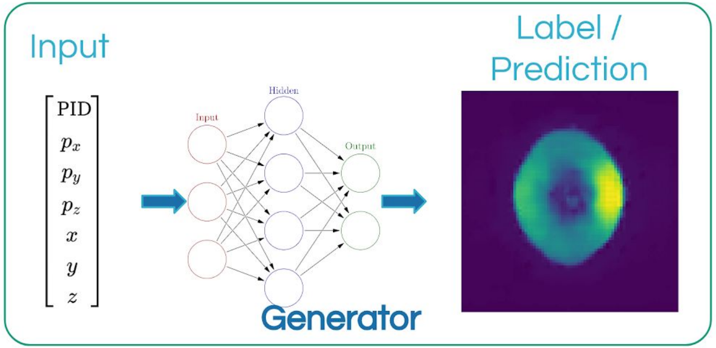


- First tests are learning physical quantities successfully
- Further work underway for consistent comparisons to fiTQun

Reconstruction with Generative CNN

- We are exploring an **alternative** approach to the more traditional "end-to-end" CNN event classification for reconstruction of water Cherenkov events.



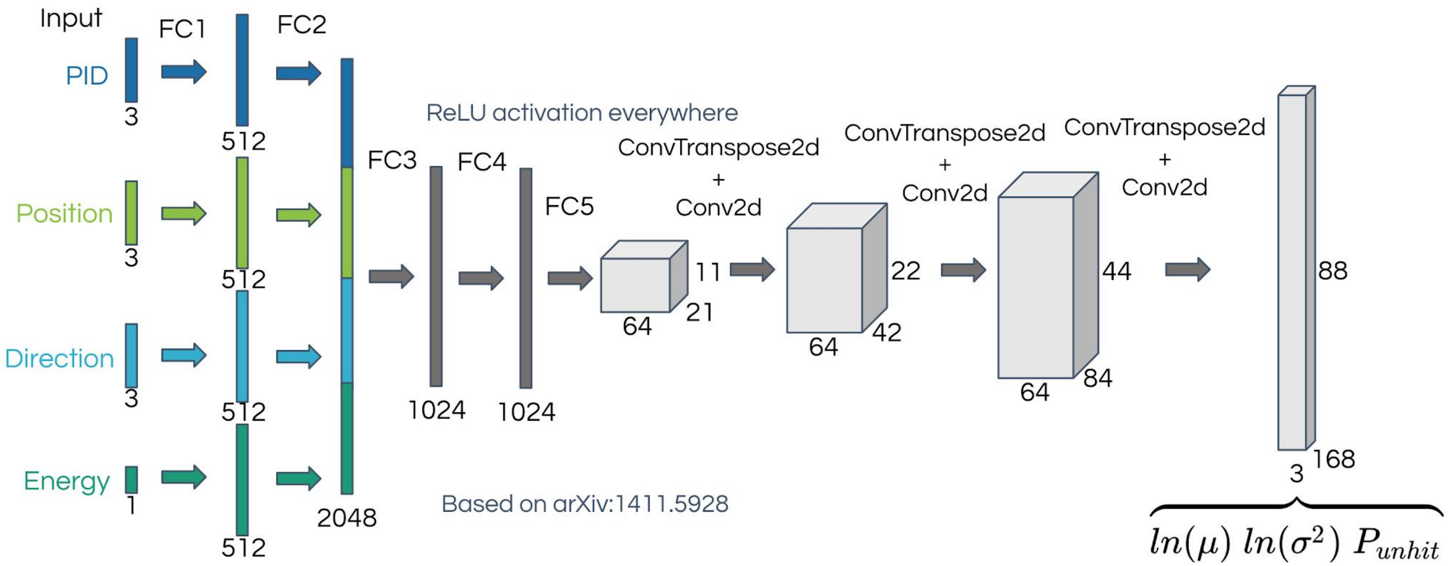


- A CNN is trained to **predict** the hit **charges** and **times** for a given set of track parameters.
- This Cherenkov ring generator can be incorporated into a **maximum-likelihood estimation** framework to form an **event reconstruction algorithm**.
  - This method is **analogous** to **FiTQun** reconstruction: the CNN replaces the parameterized charge and time pdf prediction.
- While I don't necessarily expect this method to outperform the end-to-end CNN classifier's accuracy, it has **potential advantages** in the context of **physics** analyses.

Why this might be interesting

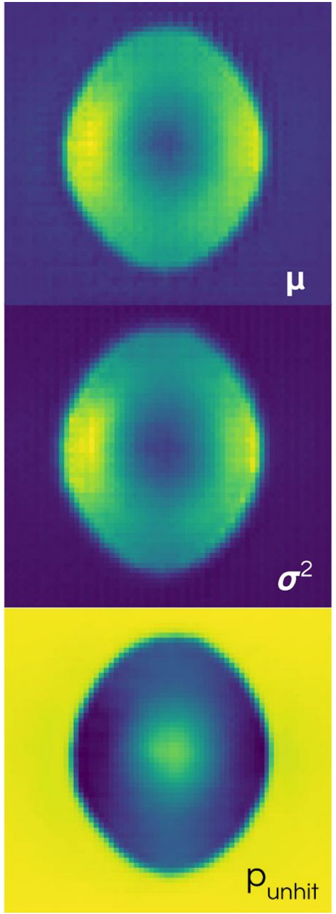
- **Single-ring** predictions can be **combined** to predict arbitrary event hypotheses.
  - E.g.: in FiTQun mean predicted charges at each PMT are added up and time pdfs are combined, weighted by charge.
- Neural network can be trained on **single-particle MC**:
  - A priori not relying on problematic neutrino and secondary **interaction models**.
  - Avoid multi-particle final states combinatorics.
- "Interesting" event topologies do not need to be defined at training stage.
  - Analyzers have **flexibility** to produce very specific event hypotheses out of single-ring predictions without having to retrain the neural network.
    - E.g.: proton decay to kaon and neutrino analysis with FiTQun specifies event with single de-excitation gamma followed (12 ns) by mono-energetic muon.
- This reconstruction approach would be a **drop-in replacement** for FiTQun.
  - Could be used with current analysis and systematic uncertainty estimation techniques, for example in the T2K and Super-Kamiokande experiments.
    - Could be a useful first step in the move towards end-to-end ML reconstruction.

Generating pdfs



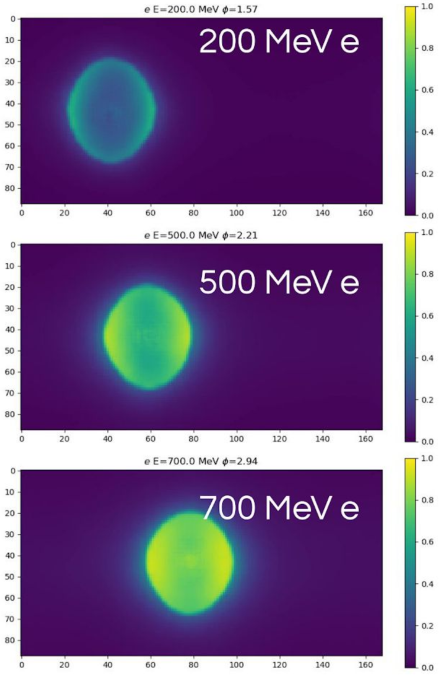
$$\text{Loss} = -ln(\mathcal{L}) = -\sum_{unhit} ln(P_{unhit}) - \sum_{hit} ln(1-P_{unhit}) - \sum_{hit} \frac{1}{2}\left[ln(2\pi\sigma^2) + \frac{(q_{obs}-\mu)^2}{\sigma^2}\right]$$

- Output is a (Gaussian) **charge pdf** and **hit probability** for **each PMT**.

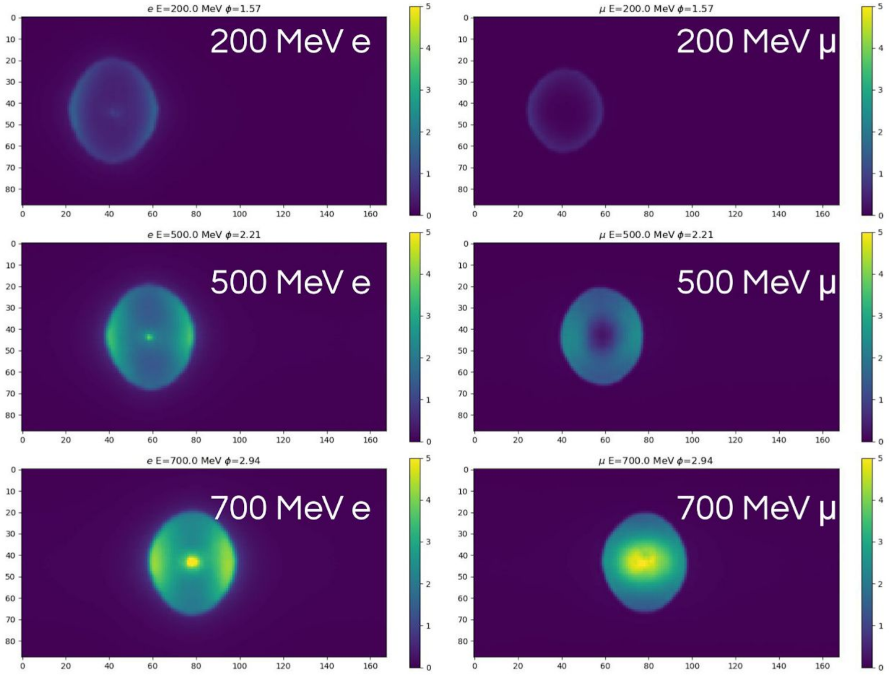


Generated ring examples

Hit probability



Hit probability x Mean charge



Generative networks

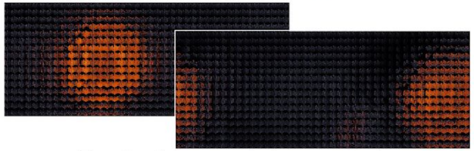
- Initially did some studies with variational auto-encoders (VAE). Interpolation results ok in energy but poor in angle. Not further pursuing at this moment.

  details: A. Abhishek et al., arXiv:1911.02369

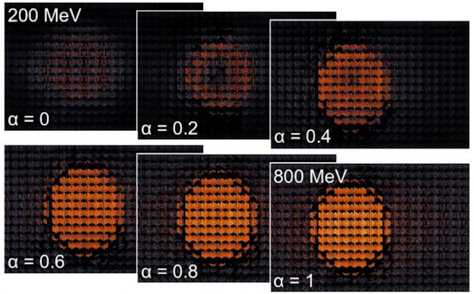
- Pursuing GANs for synthetic data generation (multiple derived tasks)

- CycleGAN* to learn transformation between MC and simulated data

  * J.Y.Zhu et al., ICCV 2017



Randomly generated new events



Interpolate between 200 MeV and 800 MeV events