A DIFFERENTIABLE SIMULATOR FOR LARTPCS
from proof-of-concept to real applications

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APC (Astroparticule et cosmologie) - Paris

June 28, 2024

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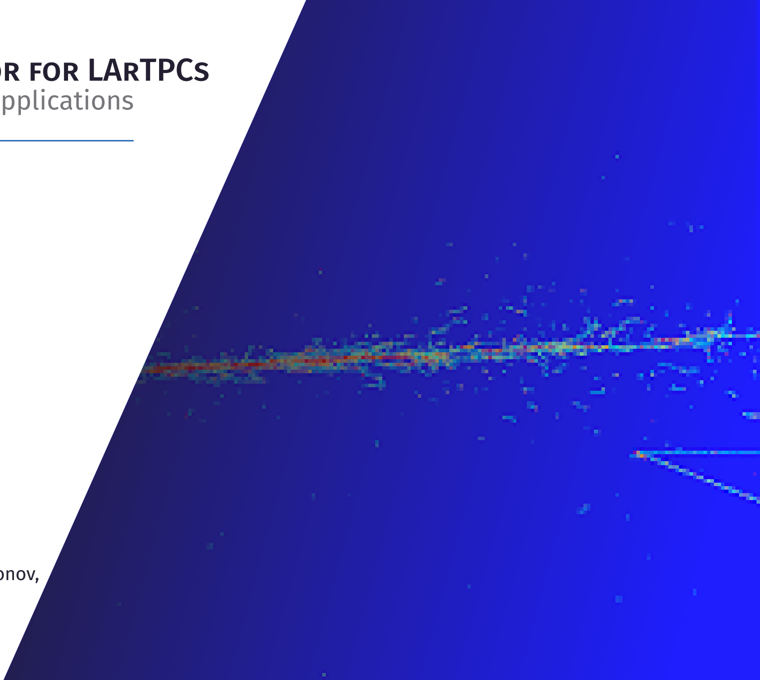


Outline

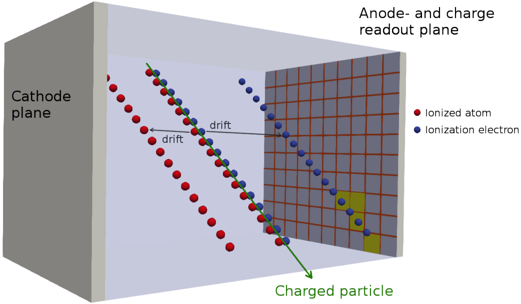
1. Motivation

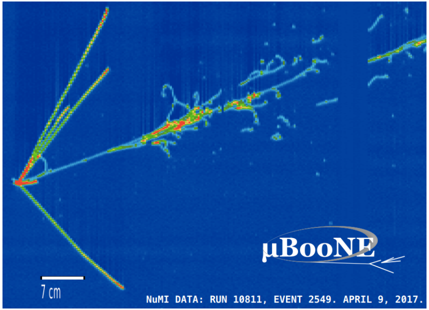
2. Recap of previous work

3. Improving the performance

4. Outlooks

LIQUID ARGON TIME PROJECTION CHAMBERS (LARTPCS)



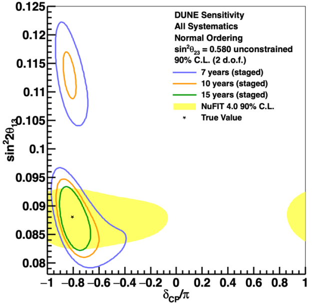


Signal production steps:

- Argon ionisation
- Ionisation electrons drifted by $\mathbf{E}$ field
- Electrons readout on anode plane

- Allows to get **precise 3D picture** of the interaction
- Relies on **multiple physical processes** $\rightarrow$ **importance of calibration**

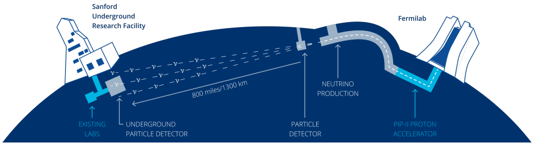
DUNE FOR PRECISION MEASUREMENTS

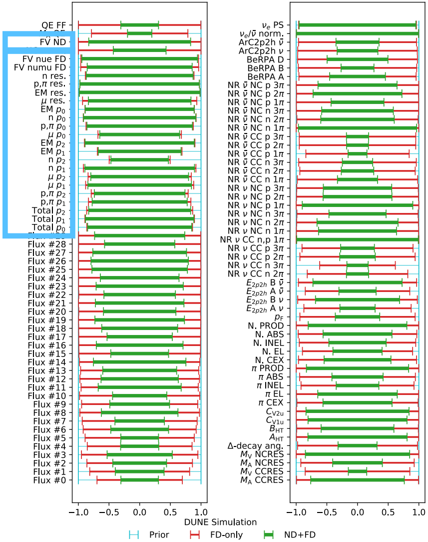


Systematics of detector modeling

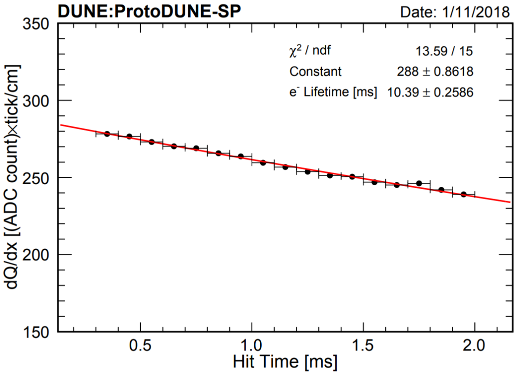
Well-understood detector modeling and calibration are vital

Eur.Phys.J.C 80 (2020) 10, 978

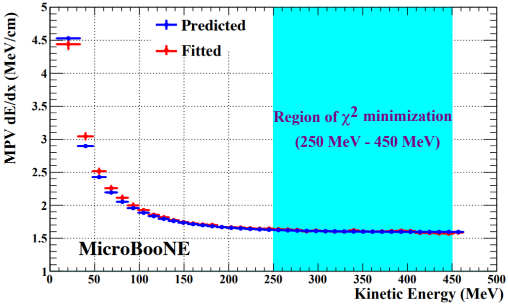




TYPICAL LARTPC CALIBRATION



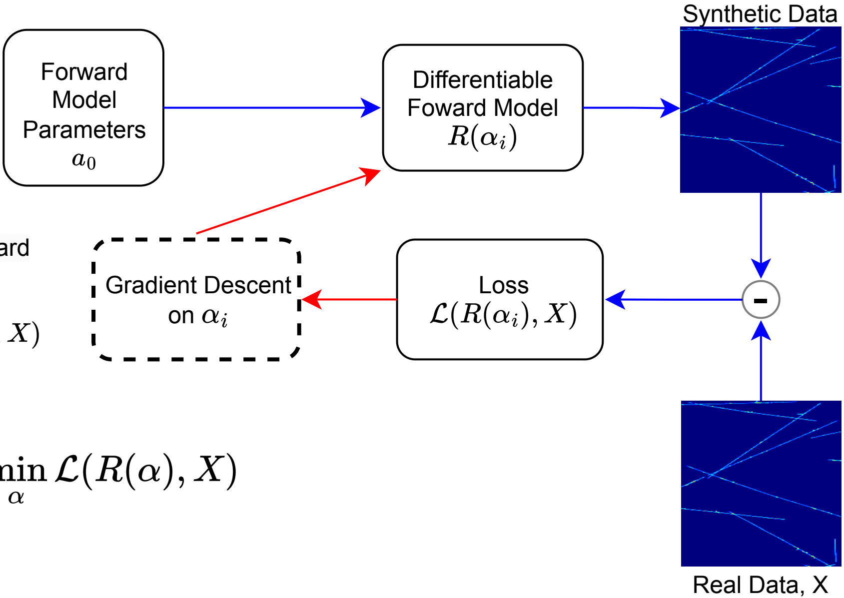
e^- lifetime calibration



Energy conversion calibration.

Calibration of the different physical parameters are typically done in **different studies**.
$\longrightarrow$ **can be simplified with a differentiable simulator**

Using gradient-based optimization



Requires forward model to be differentiable: $\nabla_{\alpha_i} \mathcal{L}(R(\alpha_i), X)$

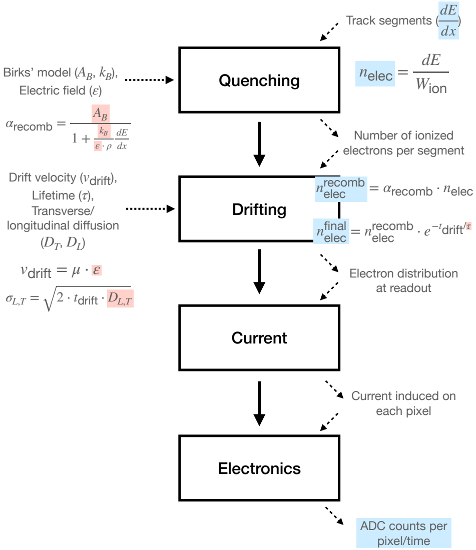
$$\alpha^* = \arg\min_{\alpha} \mathcal{L}(R(\alpha), X)$$

Starting from a non-differentiable LArTPC simulator

Our work: take existing DUNE near-detector simulation (JINST 18 P04034) and **make it differentiable.**

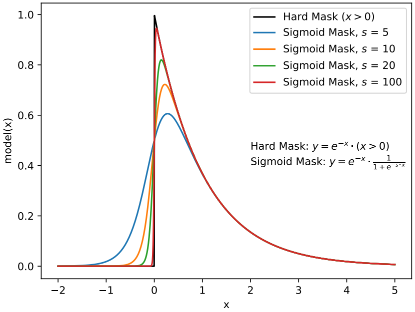
- Retain physics quality of a tool used collaboration-wide while adding ability to calculate gradient
- Demonstrate the use of this differentiable simulation for **gradient-based calibration**

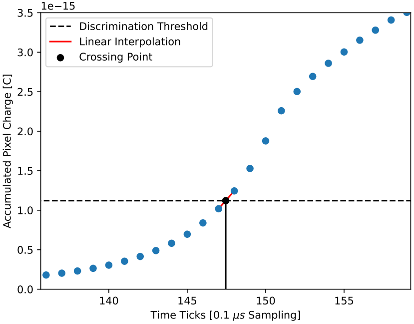
→ **How to do it practice?**



Differentiable relaxations

The base simulation contains **discrete operations** $\rightarrow$ non-differentiable.
Requires differentiable relaxations to be able to get usable gradients.





- Cuts (e.g. x > 0) $\rightarrow$ smooth sigmoid threshold
- Integer operations (e.g. floor division) $\rightarrow$ floating point (e.g. regular division)
- Discrete sampling $\rightarrow$ interpolation

Rewriting the simulator

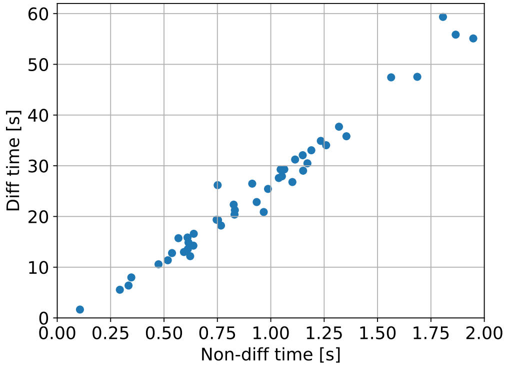
Numba code using **CUDA JIT compiled kernels** → Framework change for diff version:

- Differentiable version rewritten using EagerPy(backend agnostic)/PyTorch, which is based around tensor operations → use of autograd for automatic gradient calculations
- New version rewritten in a **vectorized** way to fit within these frameworks

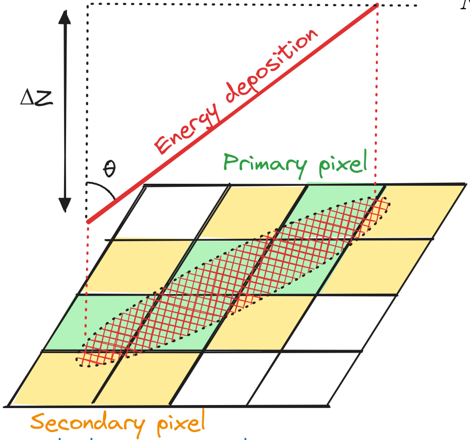
Performance drawbacks:

- Use of dense tensors to represent a sparse problem
- Moving from **CUDA JIT compiled dedicated kernel** to a **long chain of generic kernels** (vectorized operations).

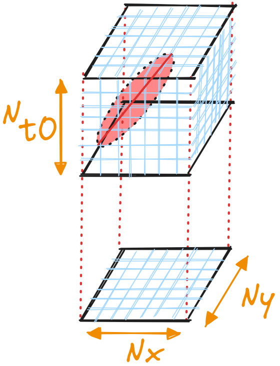
→ **also impacting memory usage**

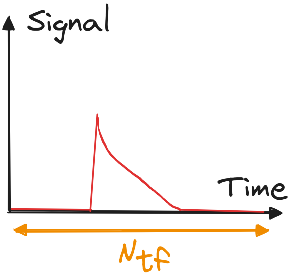


The simulator in more details



$N_{t0} \propto \sqrt{1 + \cot^2 \theta}$ $\quad N_{tf} \propto \Delta z$



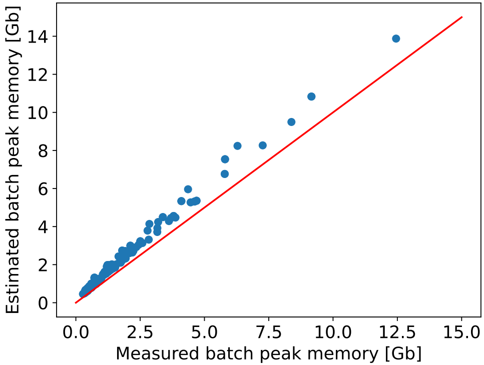


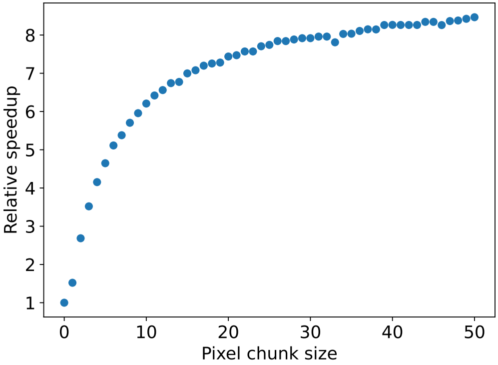
1. Calculation of N electrons
2. Estimation of charge spreading
3. Finding primary pixels
4. Finding secondary pixels
5. For each segment-pixel pair
6. Compute the intersection
7. Compute charge per voxel (Δx Δy Δt0)
8. Compute signal for all tf

MEMORY CHALLENGE

$$\mathcal{M} = \overbrace{N_{\text{segments}} \times N_{\text{pixels}}}^{\text{chunk}} \times N_{t0} \times N_{tf} \times N_x \times N_y$$

Because of the use of dense tensors, **memory** $\propto \boldsymbol{\Delta_z} \times \sqrt{\mathbf{1 + \cot^2 \theta}}$. (length in drift direction and angle) $\rightarrow$ introduced **automatic memory estimation** for each batch to estimate best pixel chunk size.



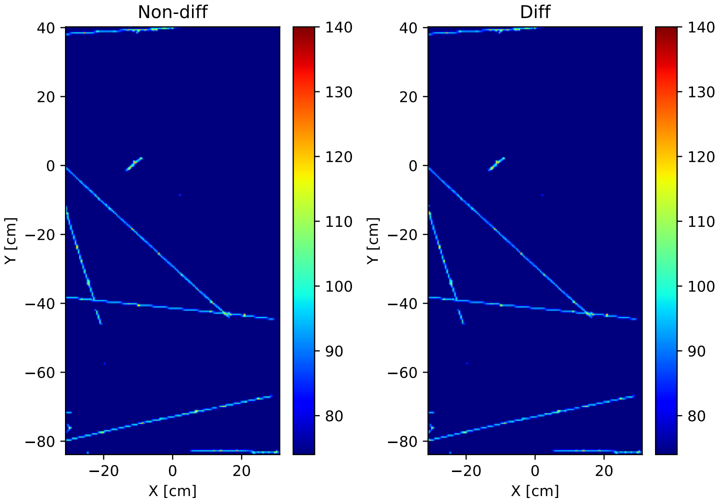


Trade-off between memory and computation time $\rightarrow$ use of gradient checkpointing

Checking the result

Checking that the **relaxations don't modify the simulator output.**

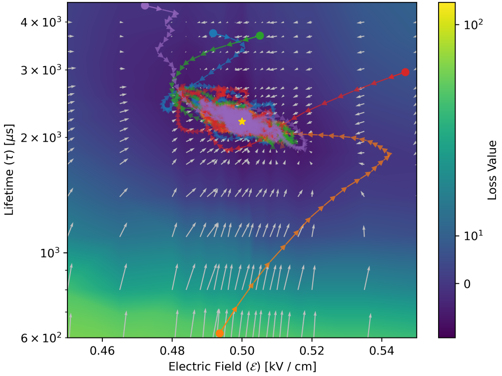
Average deviation of 0.04 ADC/pixel $\rightarrow$ well below the typical noise level of few ADCs.



Optimization of the Model Parameters

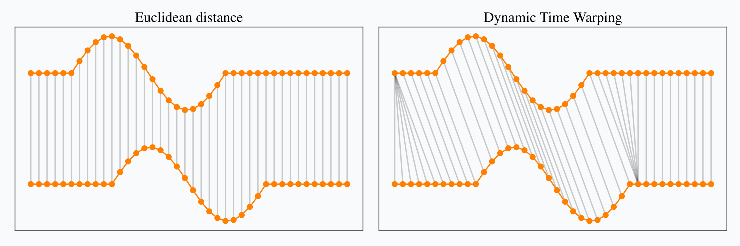
- Input particle segments (position and energy deposition): χ
- Model parameters: θ
- Differentiable simulation: $f(\chi, \theta)$
- Target data: F_{target}

1. Choose the initial parameter values θ_0
2. Run the forward simulation $f(\chi, \theta_0)$
3. Compare the simulation output and the target data with a loss function $\mathcal{L}(f(\chi, \theta_0), F_{\text{target}})$
4. Calculate gradients for the parameters $\nabla_\theta \mathcal{L}(f(\chi, \theta_0), F_{\text{target}})$
5. Update parameter values $\theta_0 \to \theta_i$ to minimize the loss
   Iterate step 2. to 5.



Optimization choices: Loss function

Loss function choice is crucial for minimization quality



https://rtavenar.github.io/blog/dtw.html

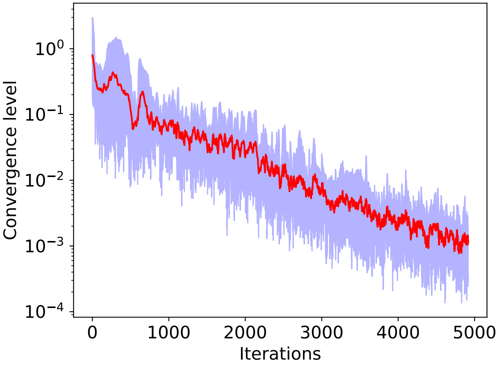
Two main ways of computing the loss:

- Comparison of 3D voxel grids of charges (x, y, t $\rightarrow$ z, q).
  - Difficulty of taking gradients through discrete pixelization.
  - Risk of flat loss if not enough overlap in distributions.
- **Considering the waveforms for each pixel (time sequence) and using Dynamic Time Warping**
  - Using a relaxed SoftDTW version that is differentiable.

Results

Mach.Learn.Sci.Tech. 5 (2024) 2, 025012

- Input sample consisting of 1 GeV simulated muon tracks
- Second sample of muons, pions and protons (1 GeV to 3 GeV)
- Geometry of a DUNE ND-LAr-prototype module: 60 cm $\times$ 60 cm $\times$ 120 cm
- Noise model available in simulator but not used.



6D simulteanous fit converging under L_∞

Doing a "closure test" based on simulated data, $F_{\text{target}} = f(\chi, \theta_{\text{target}})$:
$\rightarrow$ Fit of 6 physical parameters **simulteanously** on simulated data for multiple targets.

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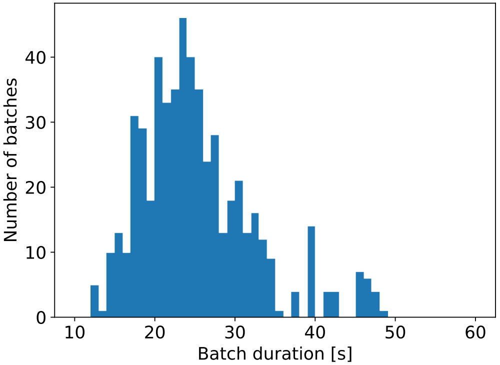
Improving the performance: why?

Current simulator performance are limiting for future applications:

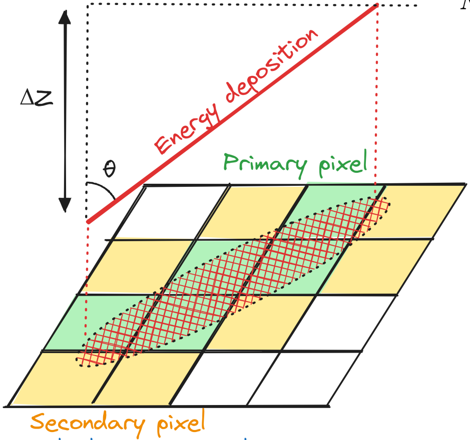
- Application to real data (Yifan pres.) $\rightarrow$ large batches and quantity of data required to mitigate the effects of electronics noise
- Being able to have more complicated physical models: inhomogeneous drift fields, space charge effect, ...
- Running the code on less demanding hardware (major limitation on memory)
- Allowing to ease uncertainty quantification: running multiple fits with different seeds, computing result on whole distributions, ...

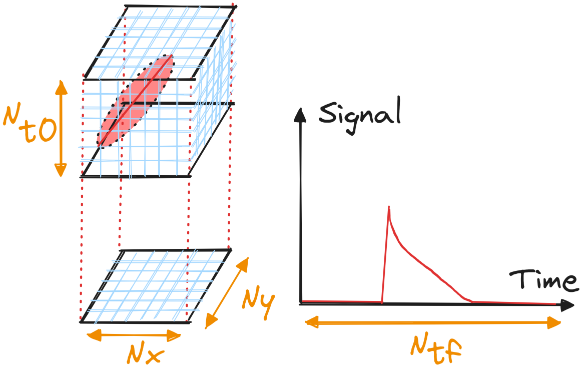


$\sim$ 25 s to process a 100 cm batch $\rightarrow$ $\sim$ 30 h for a full fit (5000 iterations)

Bottleneck of the initial code

$N_{t0} \propto \sqrt{1+\cot^2\theta}$ $\qquad$ $N_{tf} \propto \Delta z$





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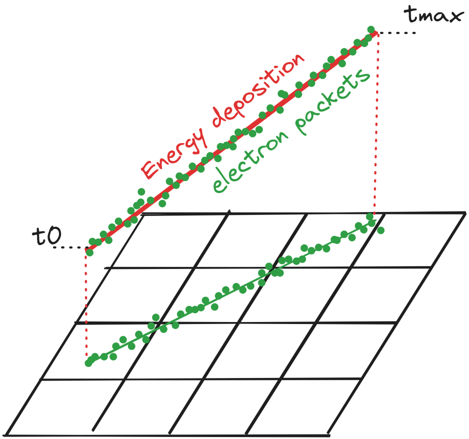
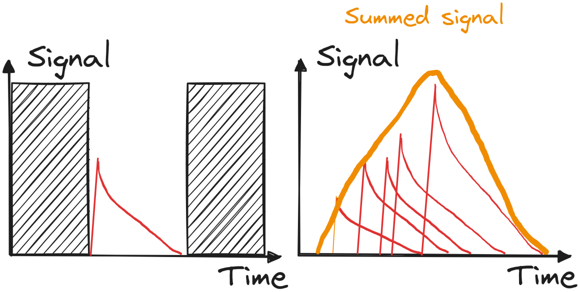
Redisigning the simulation code





1. Calculation of N electrons
2. Generation of MC e- packets
3. Get t0, x, y of e- packet
4. Get associated xpad ypad
5. For each e- packet compute waveform
6. Realign and sum waveforms per pixel

Change of framework

Benefit of the code redesign to rewrite with a new framework: JAX

Why JAX:

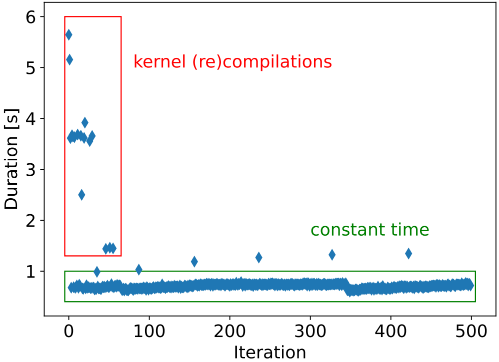
- Allows for ”easy” Just In Time kernel compilation
- Efficient calculation of the gradient calculation graph (XLA)
- Runs indifferently on CPU/GPU

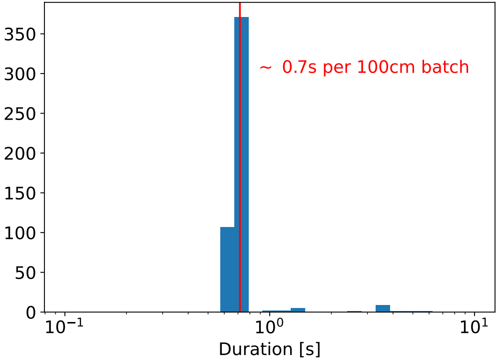
Requirements for ”easy” JIT

- No use of basic control-flow
- Loops must have a defined number of iterations
- No dynamic-shapes: the shape of all the tensors must be known at compile time $\Longrightarrow$ recompilation of kernels on each shape change

$\rightarrow$ implemented a ”shape memory” to pad inputs to nearby shapes if already compiled kernels exist to limit the number of kernel recompilations (computationally expensive)

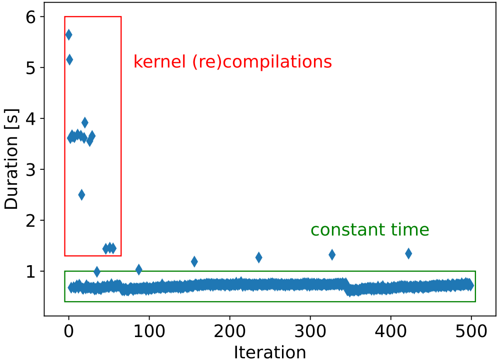
NEW PERFORMANCE

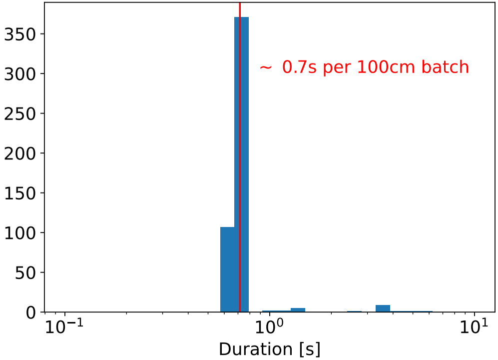




- After some iterations, kernels are already compiled for a wide range of shapes $\rightarrow$ no more overhead
- With the rework, the computation time is very strongly driven by the batch size only $\rightarrow$ almost constant computation time
- Speedup of $\sim \times 35$ $\rightarrow$ allows for a full fit in $\sim 1\,\mathrm{h}$

New performance

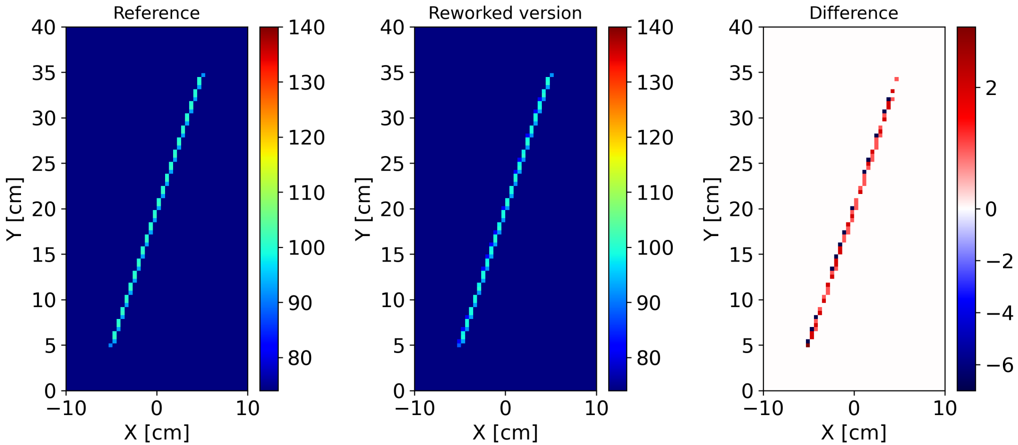




- After some iterations, kernels are already compiled for a wide range of shapes $\rightarrow$ no more overhead
- With the rework, the computation time is very strongly driven by the batch size only $\rightarrow$ almost constant computation time
- Speedup of $\sim \times 35$ $\rightarrow$ allows for a full fit in ~ 1 h
- On CPU only...

Current simulation

- Running the reworked code on GPU is $\sim 5\times$ slower than on CPU... To be investigated.
  $\rightarrow$ possibly leaves open greater computation time improvements if understood/solved
- Final checks on the correctness wrt previous simulation



Complex comparison: fixes applied wrt "Reference", $\neq$ signal simulation wrt newest larnd-sim

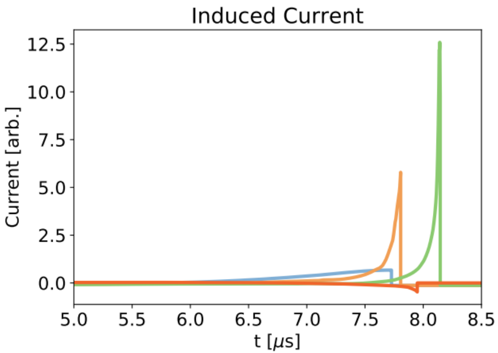
Current simulation

Old larndsim

$$I(x,y,t,t_0) = \frac{P(x,y)}{R(x,y)} e^{\frac{t_0+Q(x,y)-t}{R(x,y)}} + \frac{1-P(x,y)}{S(x,y)} e^{\frac{t_0+Q(x,y)-t}{S(x,y)}}$$

Analytical approximation of the induced current

New larndsim

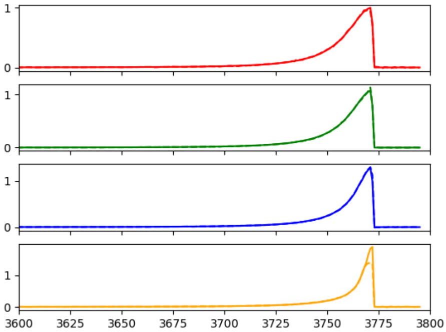


Pre-computed signals as lookup table (more accurate)

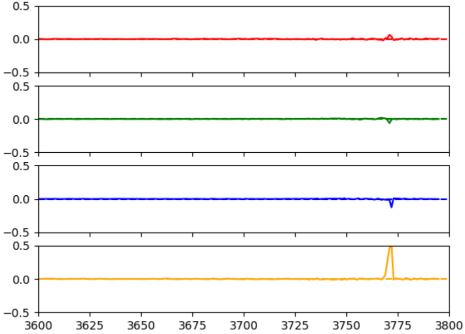
Lookup table is not differentiable, need to find another implementation

Outlooks

Ongoing work from Dan Douglas to develop a surrogate to replace the lookup table using SIREN



Waveforms: LUT (plain) and SIREN (dashed)



Residuals

Surrogate not ideal yet → probably due to the too coarse sampling of LUT

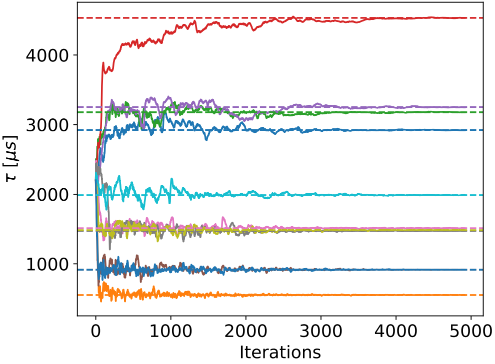
Re-running the field simulation to have a smoother input to train SIREN on

Uncertainty quantification: why?

We can make successfully make a calibration fit on simulation. How to quote an uncertainty on the obtained value?

Several uncertainties we might want to take into account:

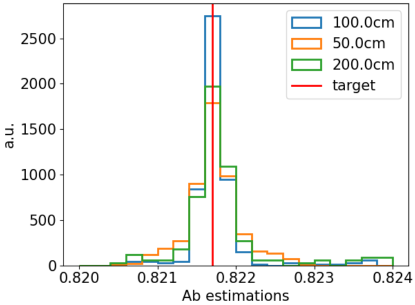
- Uncertainty on the physical parameters / physical processes
- Uncertainty on the true energy deposits (inaccessible in data)
- Stochasticity due to noise



UQ: Uncertainty on the calibrated parameters

Estimating the uncertainty on the calibrated parameters:

- Computing the Hessian matrix to estimate the parameters error (easily accessible in a differentiable simulator)
- Profiling the fitted value after convergence
- Running multiple fits in parallel and compare the convergences (ensembling)



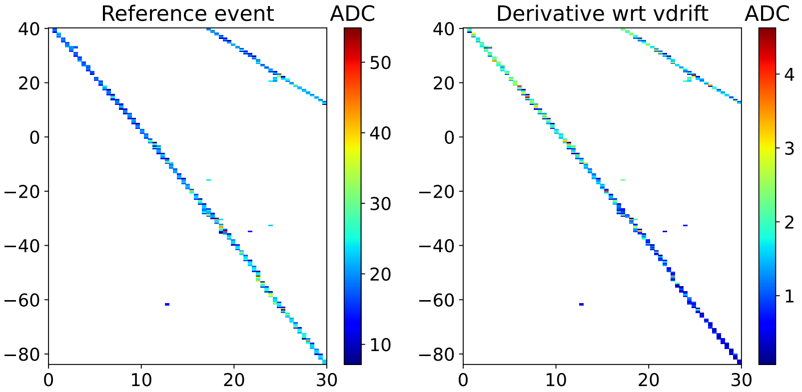
$$\mathbf{H}_f = \begin{bmatrix} \dfrac{\partial^2 f}{\partial x_1^2} & \dfrac{\partial^2 f}{\partial x_1\,\partial x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_1\,\partial x_n} \\[2.2ex] \dfrac{\partial^2 f}{\partial x_2\,\partial x_1} & \dfrac{\partial^2 f}{\partial x_2^2} & \cdots & \dfrac{\partial^2 f}{\partial x_2\,\partial x_n} \\[2.2ex] \vdots & \vdots & \ddots & \vdots \\[2.2ex] \dfrac{\partial^2 f}{\partial x_n\,\partial x_1} & \dfrac{\partial^2 f}{\partial x_n\,\partial x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_n^2} \end{bmatrix}.$$

$$E = \begin{bmatrix} \sigma_1^2 & \sigma_{12}^2 & \cdots \\ \sigma_{21}^2 & \sigma_2^2 & \\ \vdots & & \ddots \end{bmatrix} = 2H_f^{-1}$$

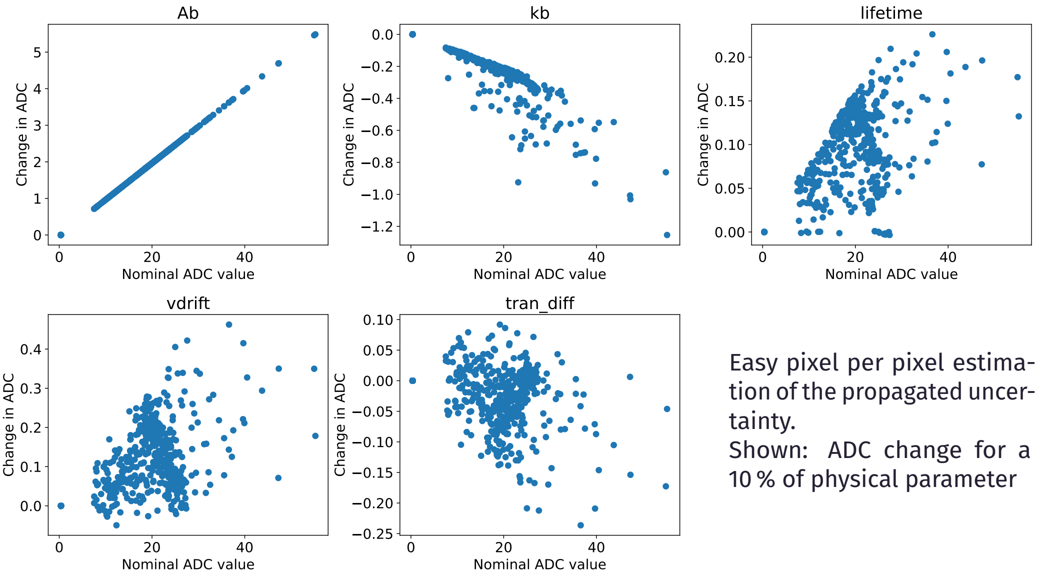
UQ: Linear error propagation

$$q(x_i) \implies \sigma_q^2 = \sum_i \left(\frac{\partial q}{\partial x_i} \sigma_{x_i} \right)^2$$

Linear error propagation allows for an estimation of the output uncertainty based on the input parameters uncertainties $\rightarrow$ Only requires the already available derivatives



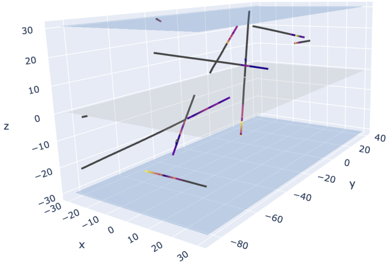
UQ: Linear error propagation



Easy pixel per pixel estimation of the propagated uncertainty.
Shown: ADC change for a 10 % of physical parameter

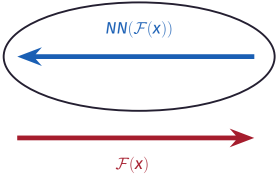
GOING FURTHER

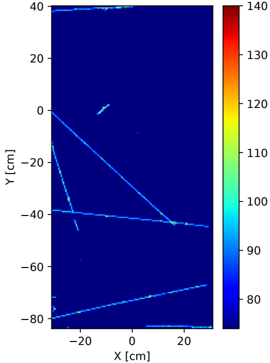
Combining our differentiable simulator with an inverse mapping would allow for direct model constraining, fully data driven: $\mathcal{L}_{CC} = (\mathcal{F}(NN(y_{\text{data}})) - y_{\text{data}})^2$



Energy deposits $\mathrm{d}E/\mathrm{d}x$
(inaccessible in data)

Inverse mapping step to developp





Detector readout

Might allow to improve the calibration by reconstructing the true energy deposits → important role of uncertainties (see Dan's talk today)

Conclusions

Shown here:

- Proof of concept for the calibration of a LArTPC using a differentiable simulator.
- Multidimensional fit converging correctly on simulated data with the differentiable simulator.
- Simulator rewriting allows to reach way better performance $\rightarrow$ will be important for application to real data

Upcoming challenges:

- Applying this framework to real data (DUNE 2x2 ND data) $\rightarrow$ see Yifan's talk
- Fitting more physical parameters (such as Efield map)
- Uncertainty quantification and propagation
- Inverse problem solving in the future

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June 28, 2024

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