Simultaneous Multi-effect Calibration in LArTPCs with Differentiable Simulation

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NPML

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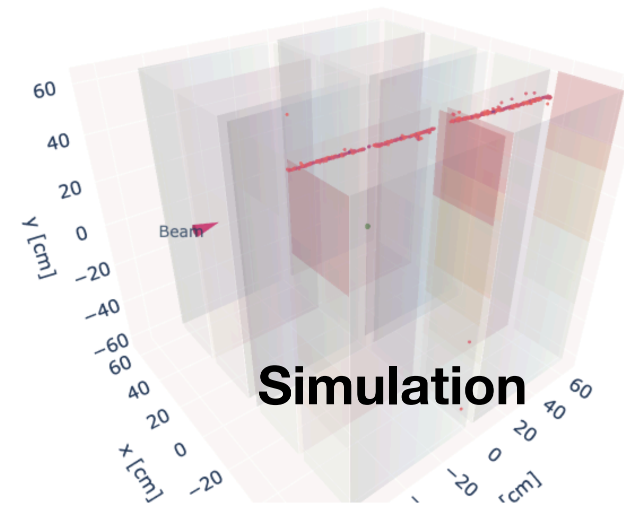
Detector Calibration with Differentiable Simulation

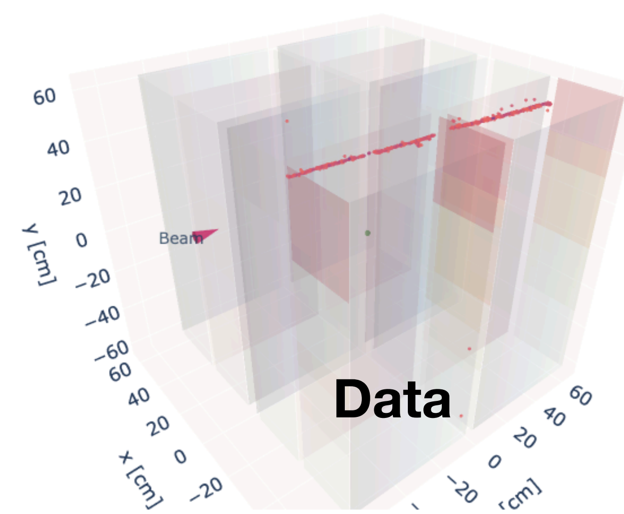
Calibration

Detector modeling parameters θ

$$\frac{dL}{d\theta}$$



Loss



Particle input → **Detector simulation**

Introduce differentiability
in explicit physic modelings

- Interpretable differentiable physics modeling
- Efficient calibration by gradient-based optimization
- Multi-effect calibration with correlations
- Simulation fidelity

[Mach. Learn.: Sci. Technol. 5 025012]

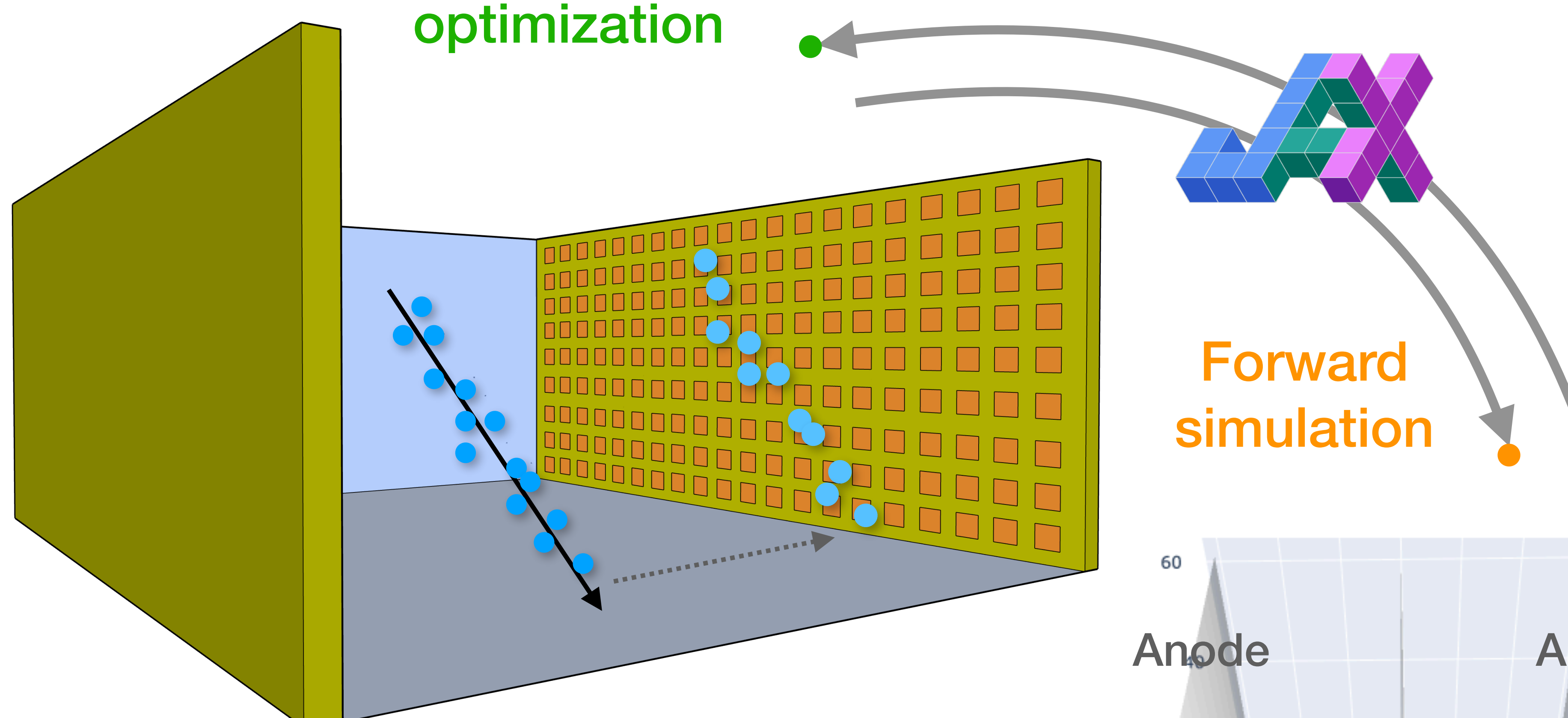
This LArTPC Differentiable Simulation

Detector simulation

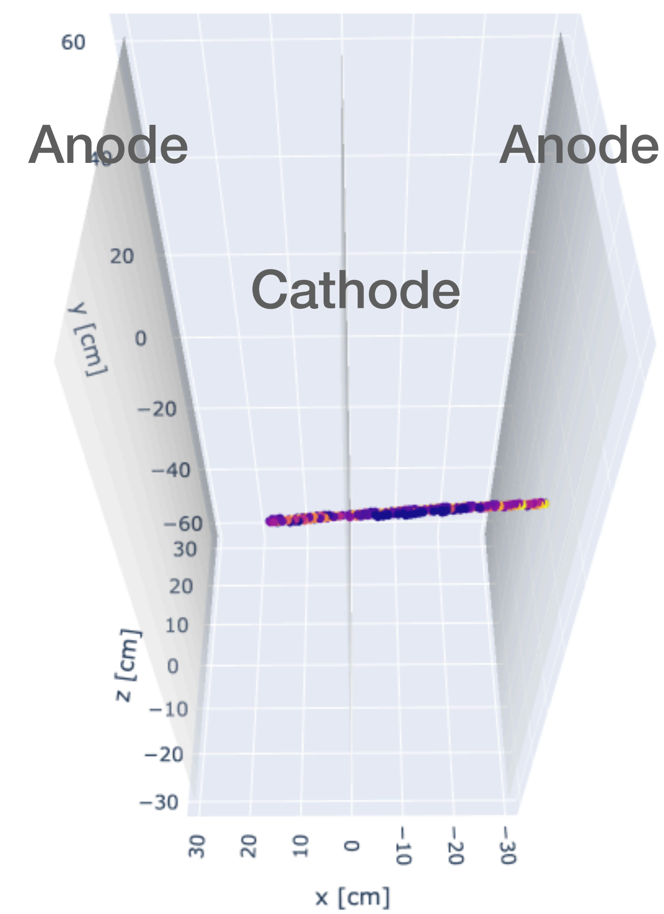
1. Quenching
2. Drifting
3. Current
4. Electronics

Gradient-based optimization

Auto differentiation



Forward simulation



6 detector modeling parameters

A_B	k_B	$\mathcal{E}$	D_L	D_T	τ
1	1	1,2,3	2,3	2,3	2

Roadmap

Gradients

Model completeness

Parameter relationships

Simulation efficiency

Calibration input

Loss

Keep the Gradients Flow

D_L	D_T
2,3	2,3

1. Quenching
2. Drifting
3. Current
4. Electronics

Gradient

Loss

Induction charge response

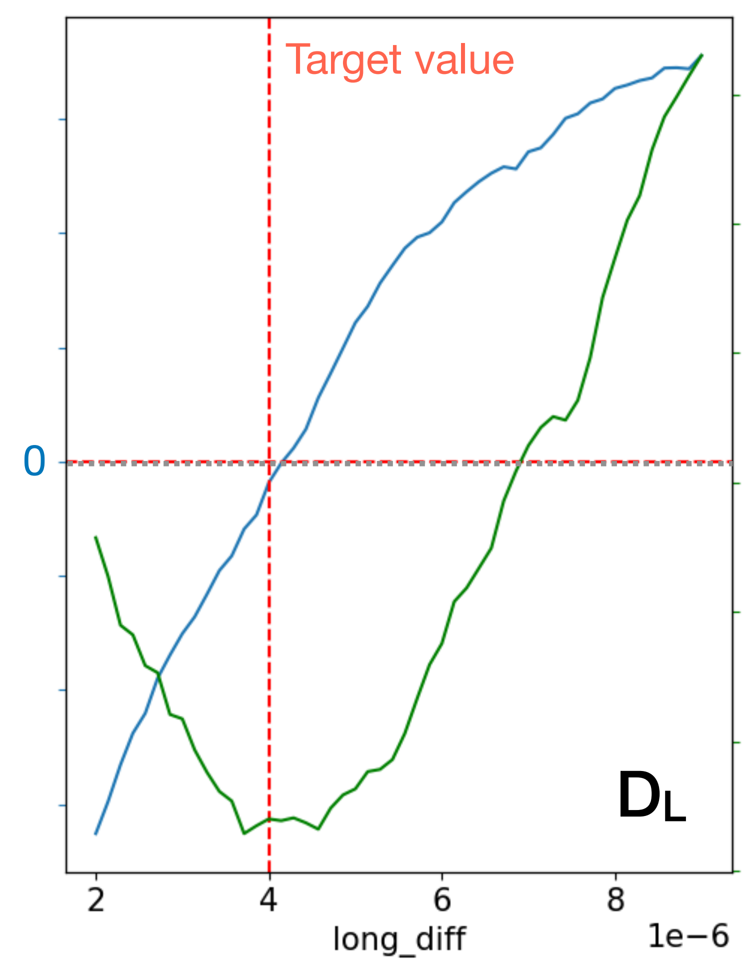
When diffusion parameters met a look-up table

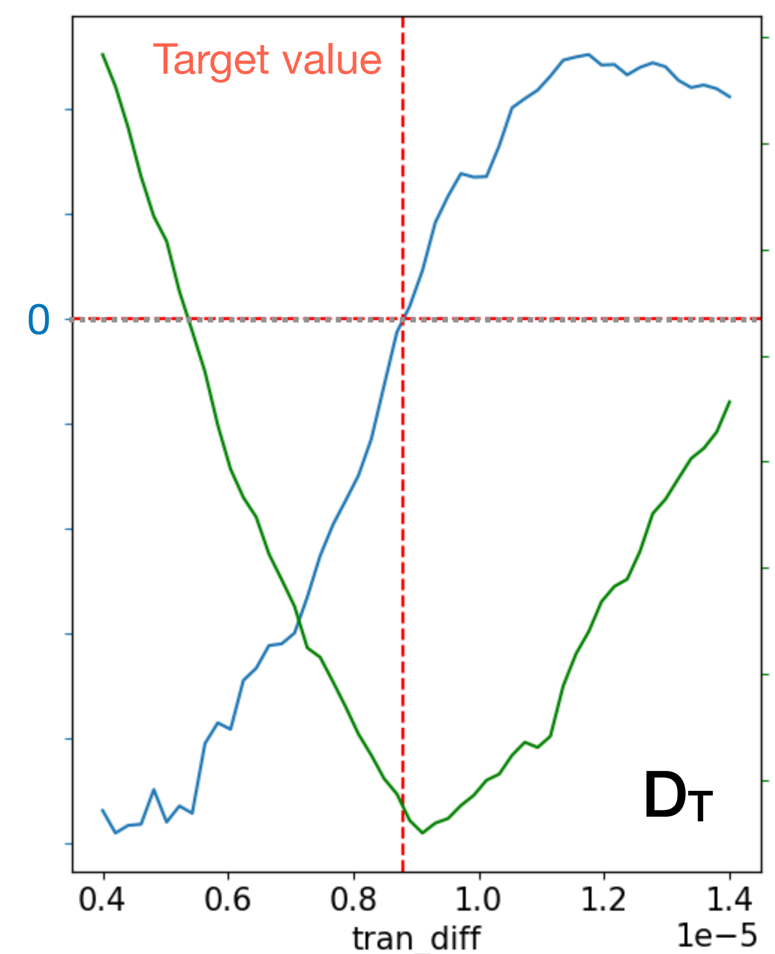
Sampling Discrete

Gradients on D_L, D_T

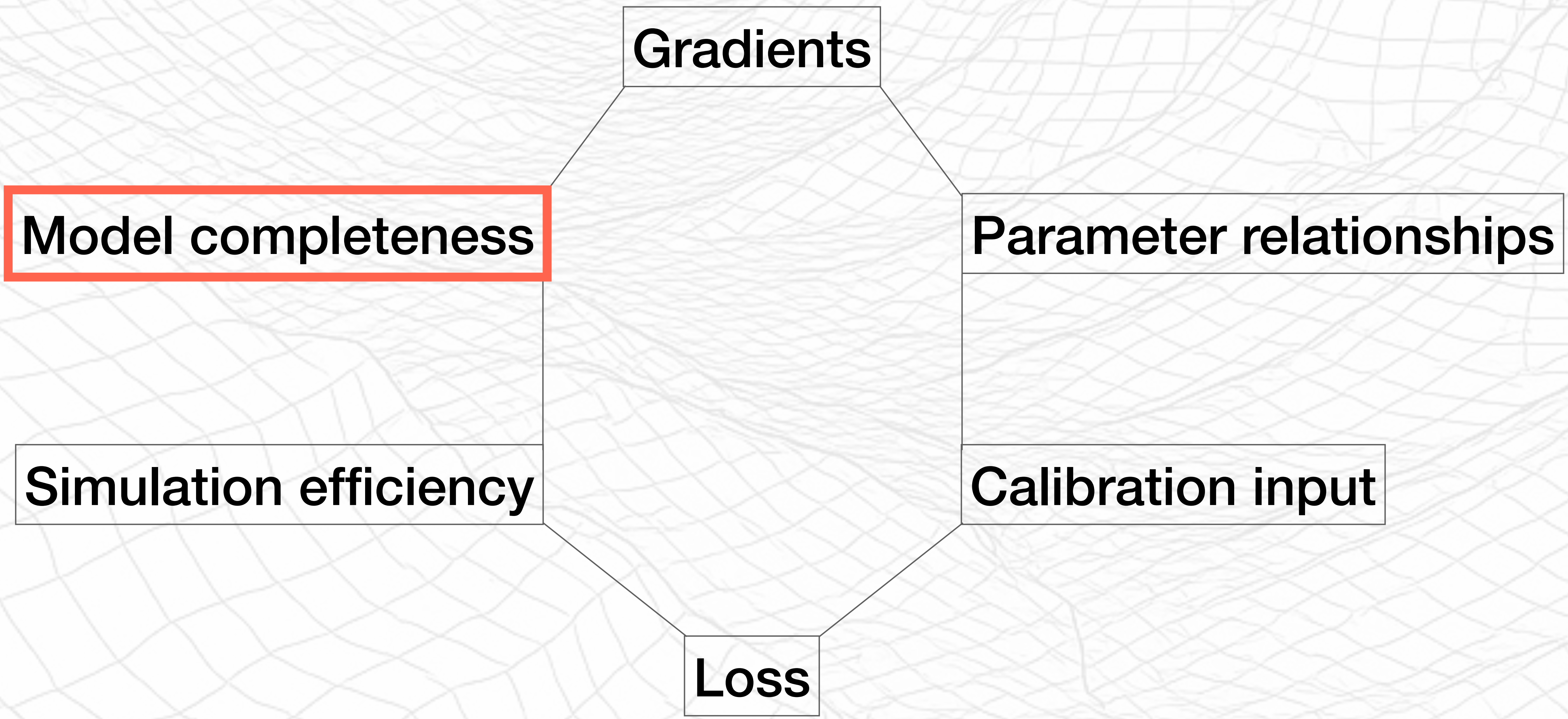
Convert Monte Carlo sampling into distributional weights

- D_L 1D Gaussian convolution + quadratic interpolation
- D_T 2D Gaussian convolution + finer binning





Roadmap


Gradients
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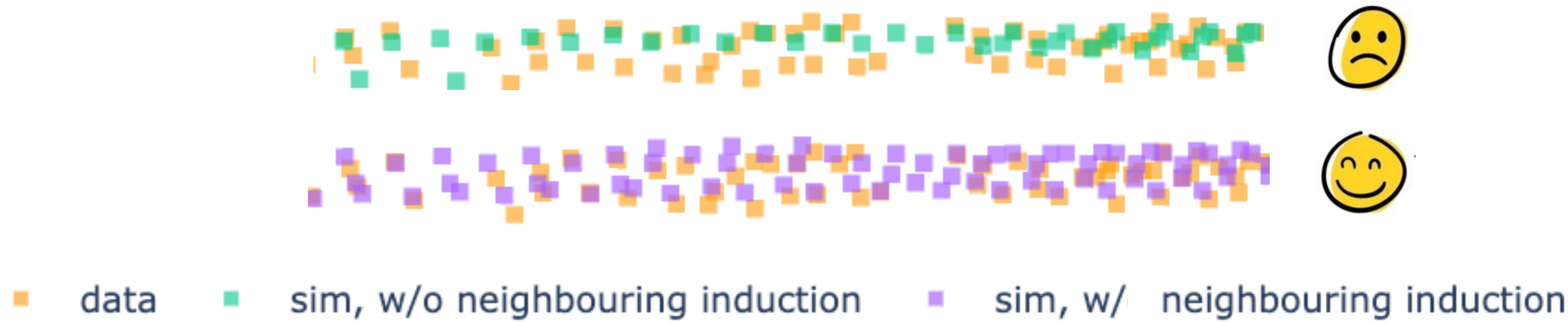
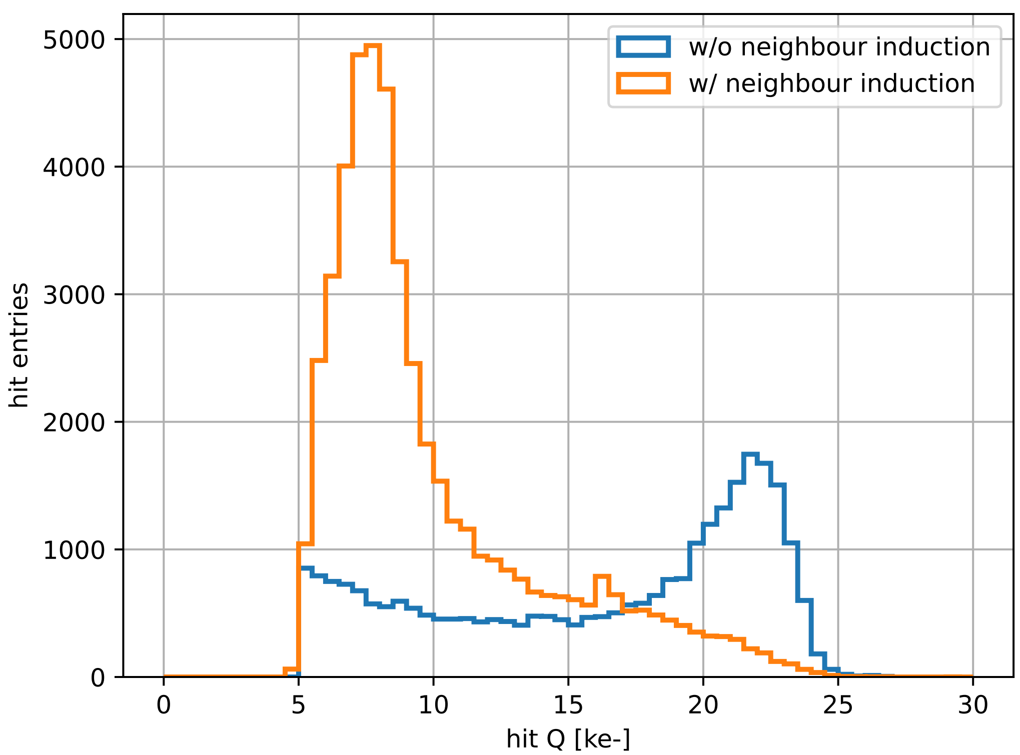
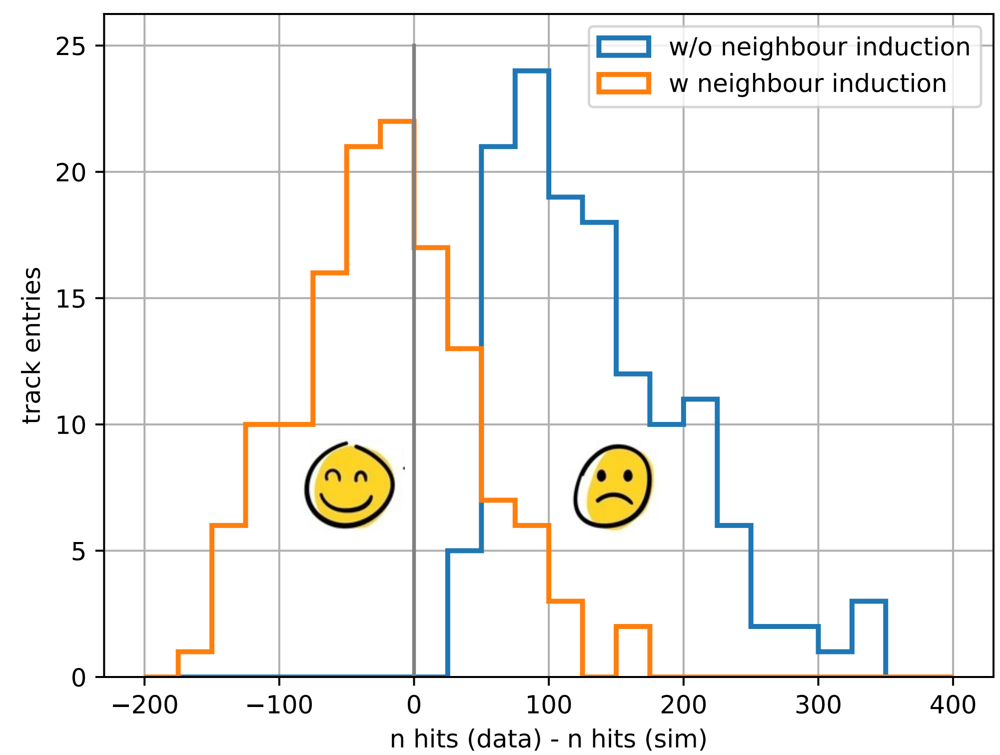
Model Completeness

Differentiable simulation used in calibration should be complete models

Through-going muons



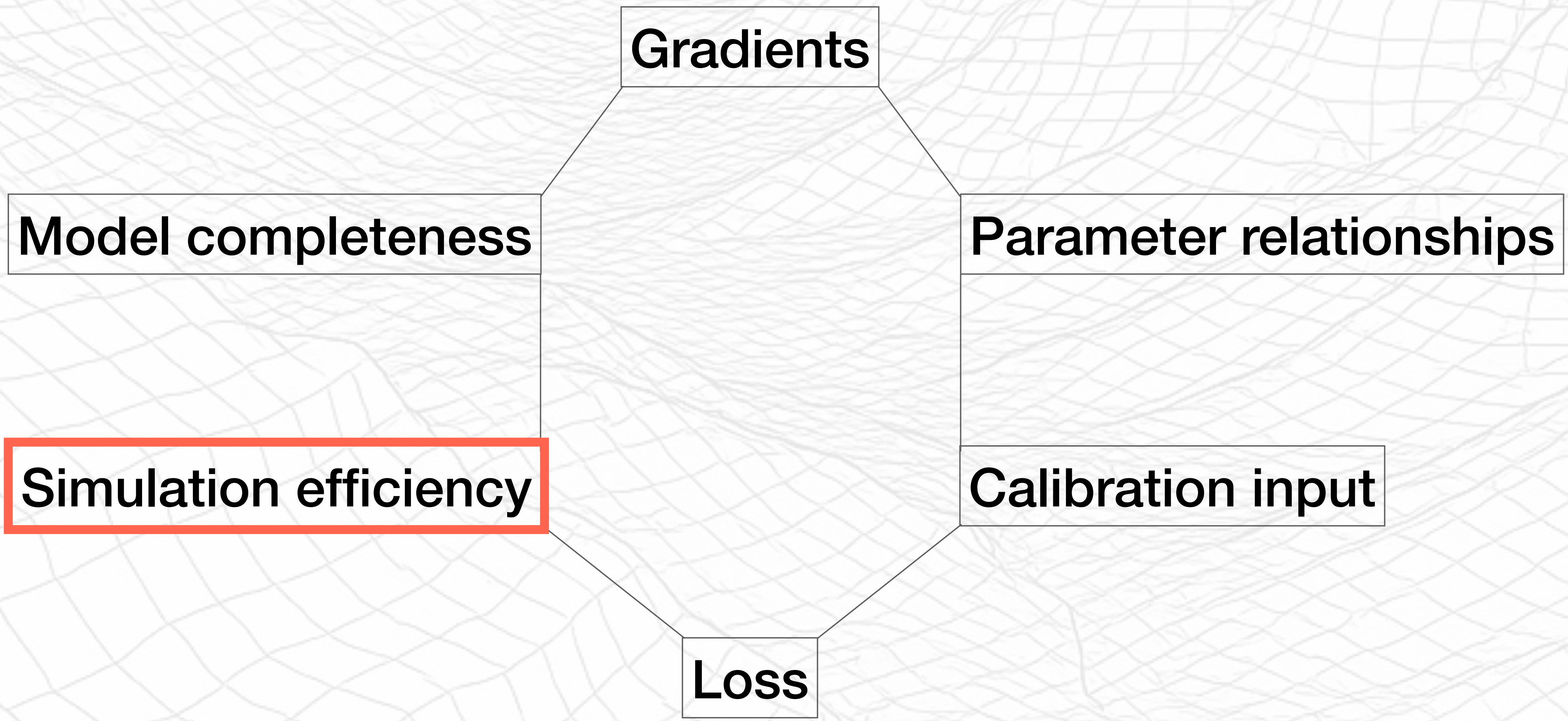




Pixel-by-pixel thresholds to be implemented in the models

"Data" on this slide is only for illustration

Roadmap


Gradients
Model completeness
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Simulation efficiency
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Loss

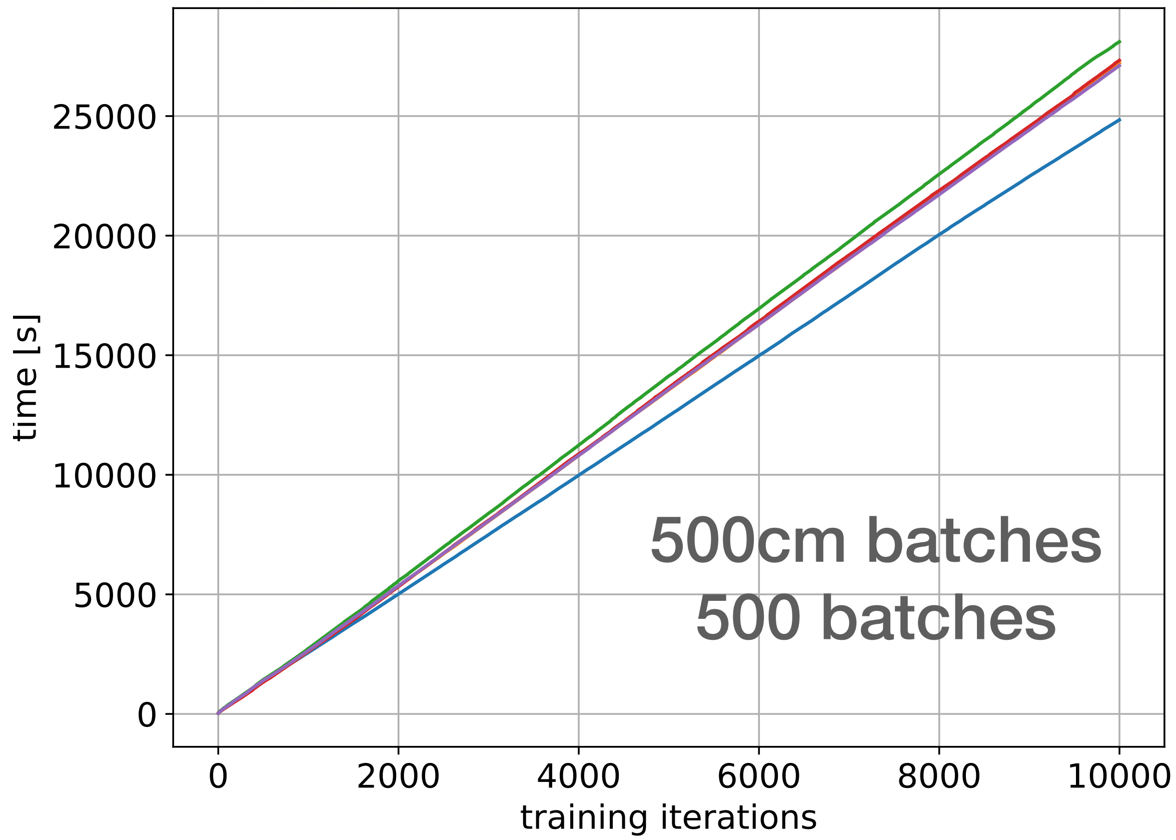
Simulation Efficiency

Simulation efficiency is crucial for real experimental applications!

Input data are segmented into 0.01 cm
One batch can fit ~600 cm (on 40 GB A100)
Run time differs slightly on parameter values

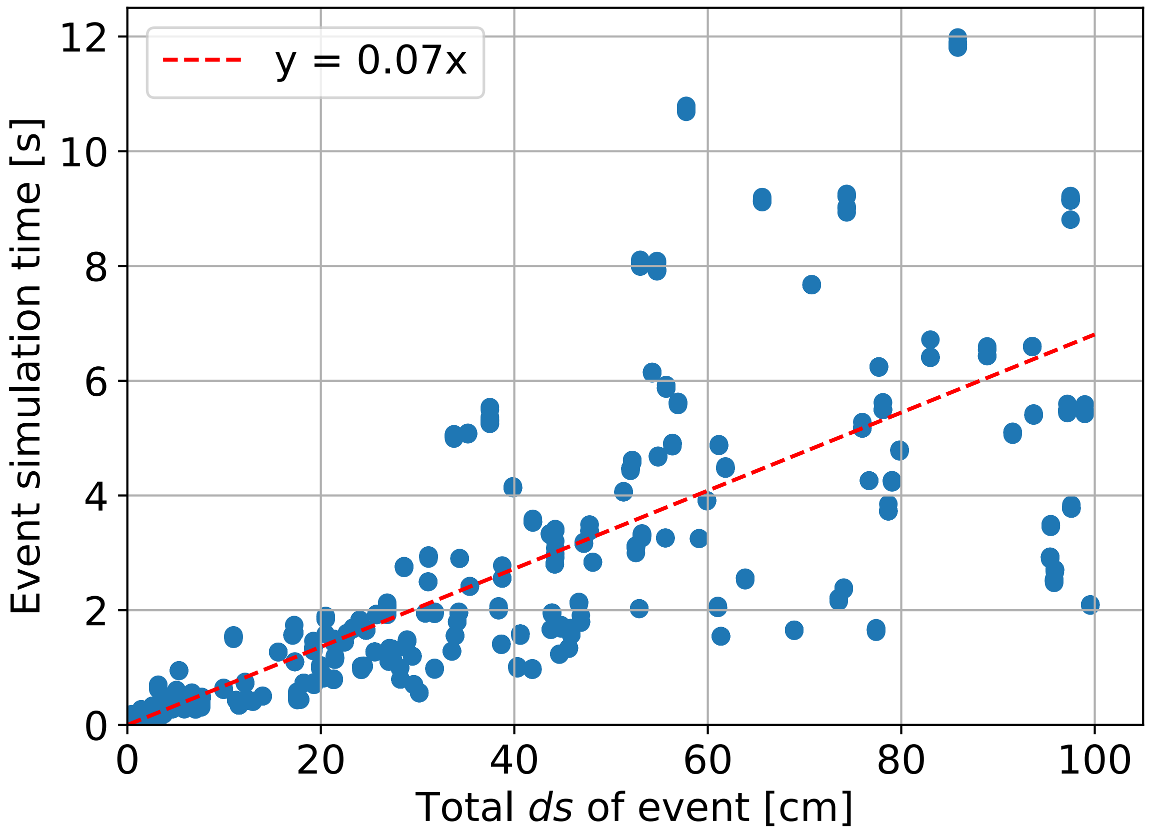
Non differentiable version
~5.6s per 500 cm

~2.6s per 500 cm



PyTorch

~35s per 500 cm



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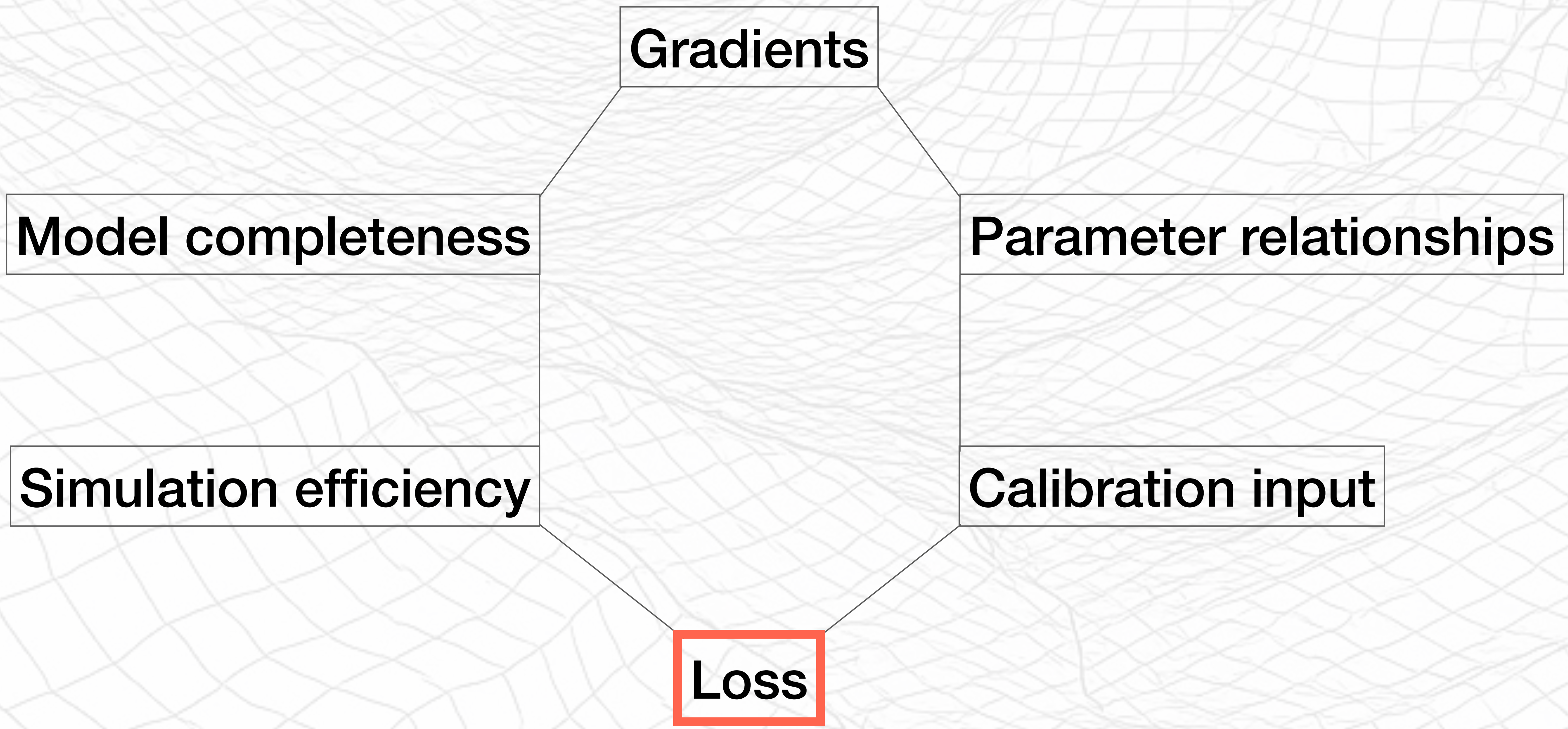
Roadmap


Gradients
Model completeness
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Loss

Loss Functions

For the calibration, the loss compares the simulation hits and data hits

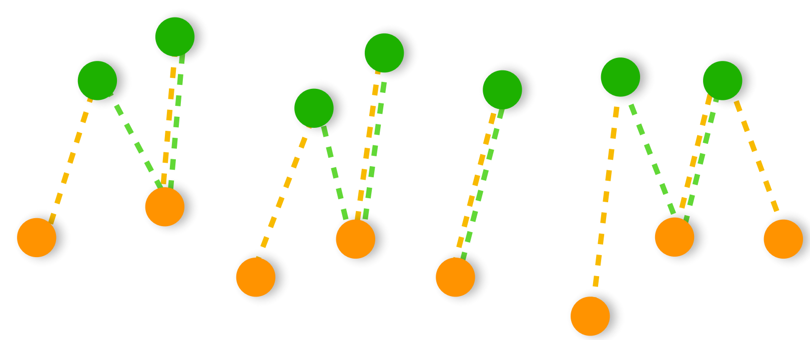
$$\nabla_\theta \mathcal{L}(f(\chi, \theta_0), F_{\text{target}}) \qquad \theta_0 \rightarrow \theta_i$$

Differentiability | Sensitivity

Point matching

Chamfer, Soft DTW

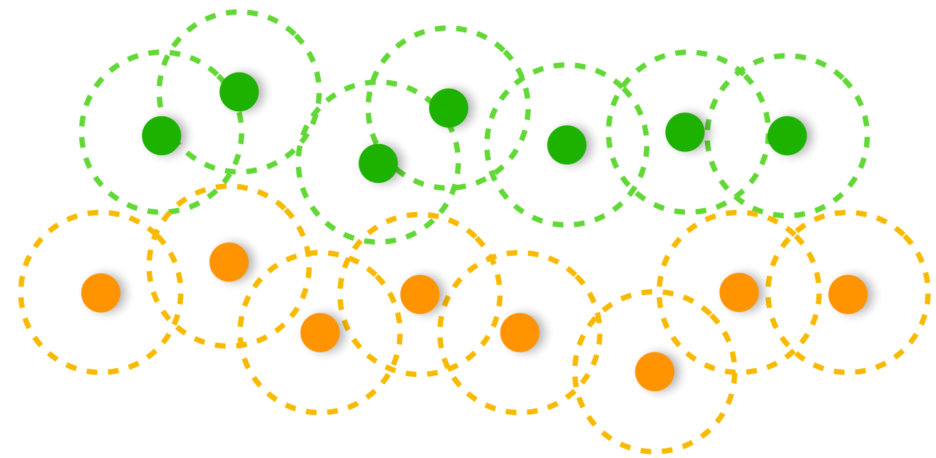
$$\mathcal{L}(f,F) = \frac{1}{|f|}\sum_{s\in f}\min_{t\in F}||s-t||^2 + \frac{1}{|F|}\sum_{t\in F}\min_{s\in f}||t-s||^2$$

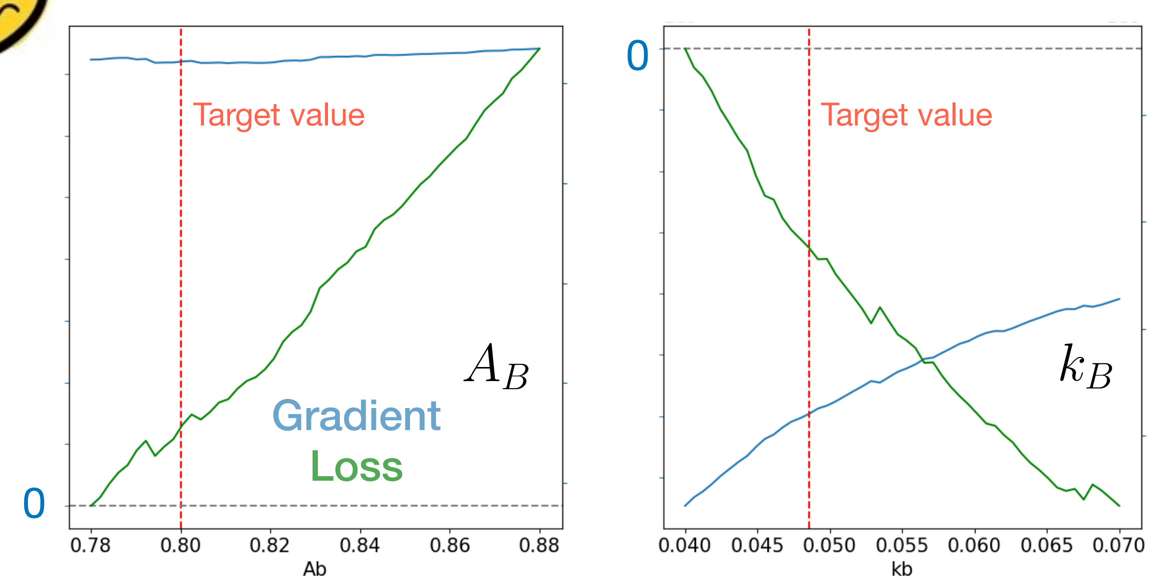


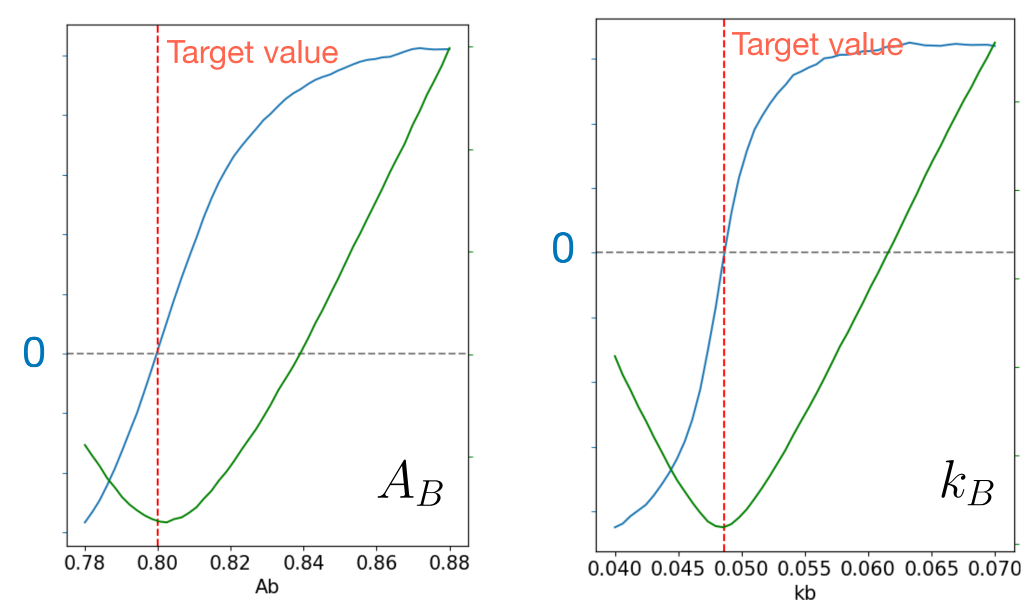
Distribution matching

Maximum Mean Discrepancy (MMD)

$$\mathcal{L}(f,F) = \mathbb{E}_{s\in f}[k(s,s)] - 2\mathbb{E}_{s\in f, t\in F}[k(s,t)] + \mathbb{E}_{t\in F}[k(t,t)]$$







Roadmap

Gradients

Model completeness

Parameter relationships

Simulation efficiency

Calibration input

Loss

Calibration Input

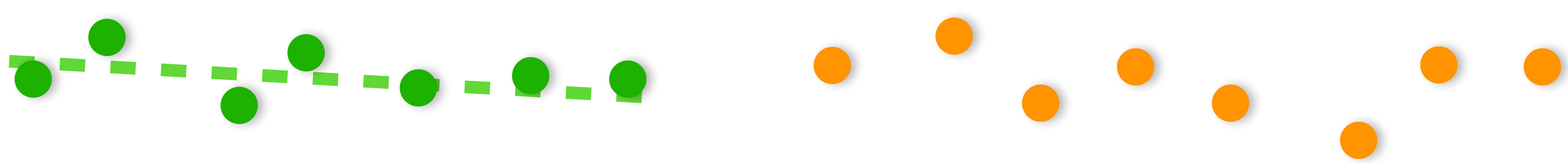
$$\underbrace{f(\underline{\chi}, \theta)}, \underbrace{F_{\text{target}}}$$

$$\mathcal{L}(f(\chi, \theta), F_{\text{target}})$$

χ

dE/dx, x, y, z

$f(\chi, \theta)$



F_{target}

Generation 1 of the Closure Tests

$$\mathcal{L}(f(\chi,\theta), \underline{F_{\text{target}}}) \rightarrow \mathcal{L}(f(\chi,\underline{\theta}), \underline{f(\chi,\underline{\theta_{\text{target}}})})$$

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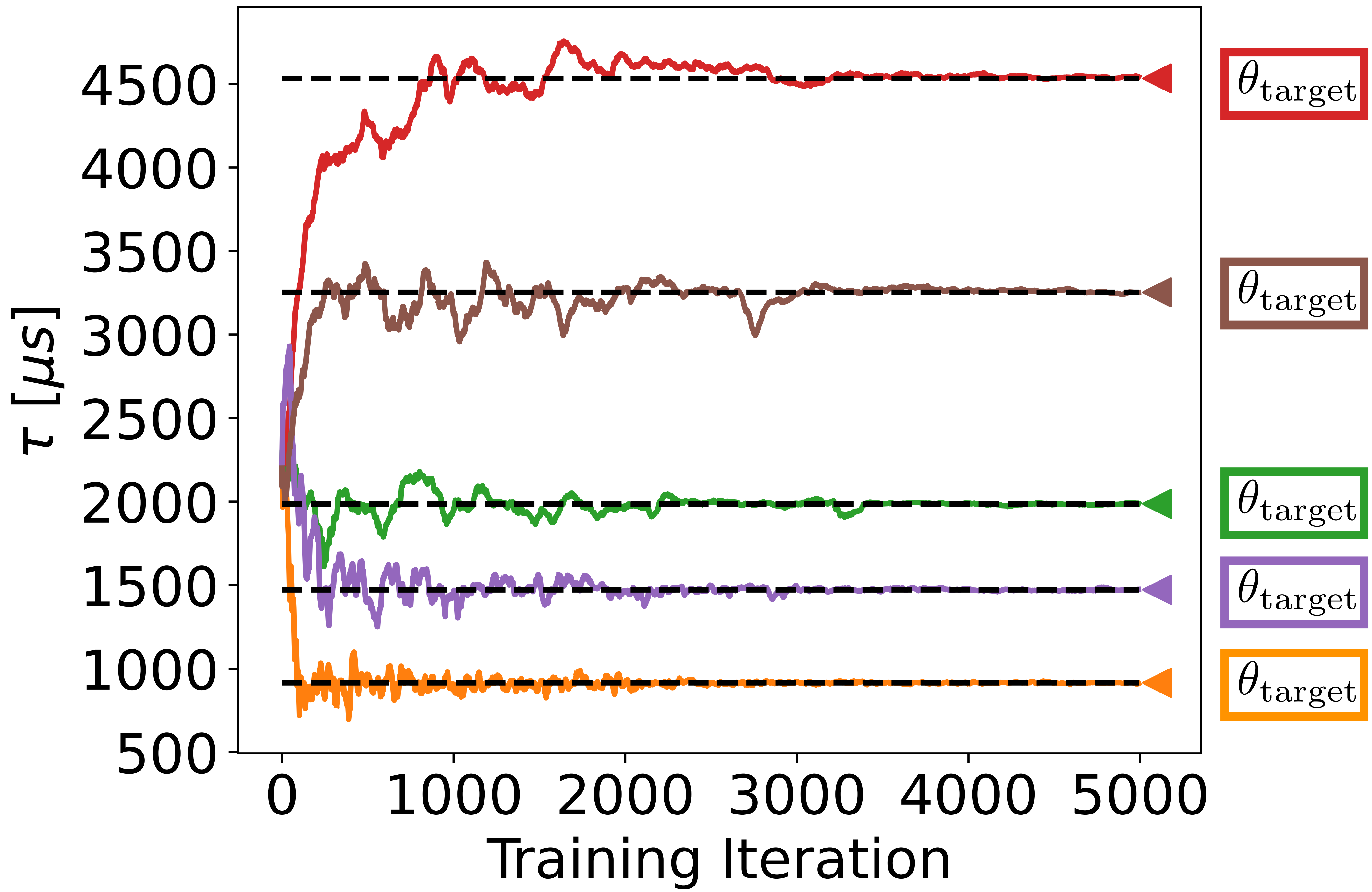
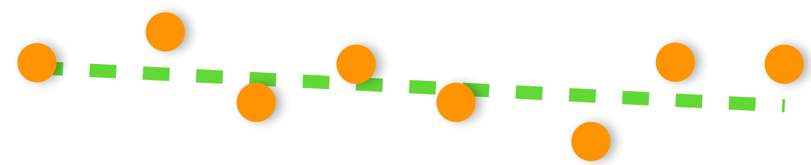


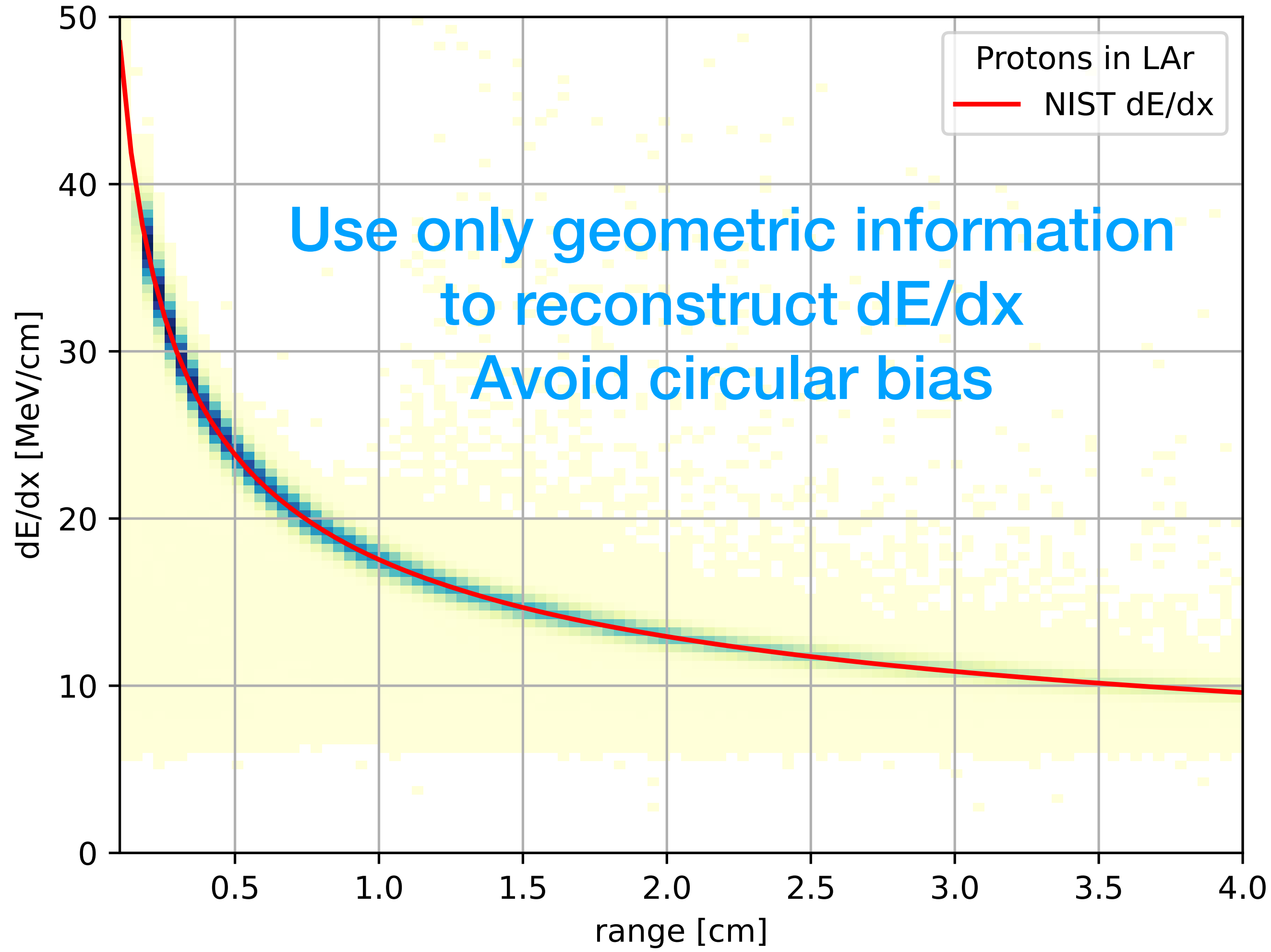
Reconstruct Simulation Input

$$\mathcal{L}(f(\chi, \theta), F_{\text{target}})$$

dE/dx x, y, z



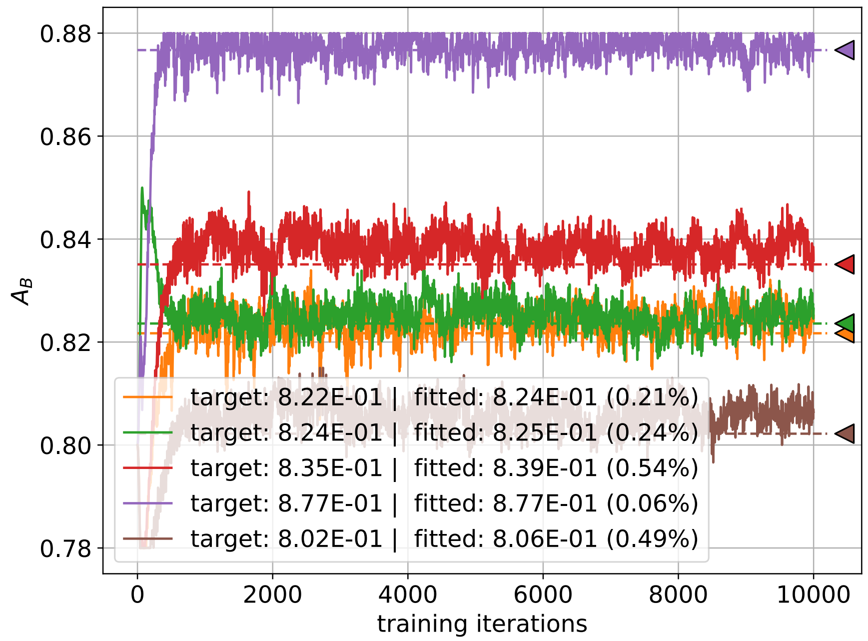
Stopping protons **Stopping muons**



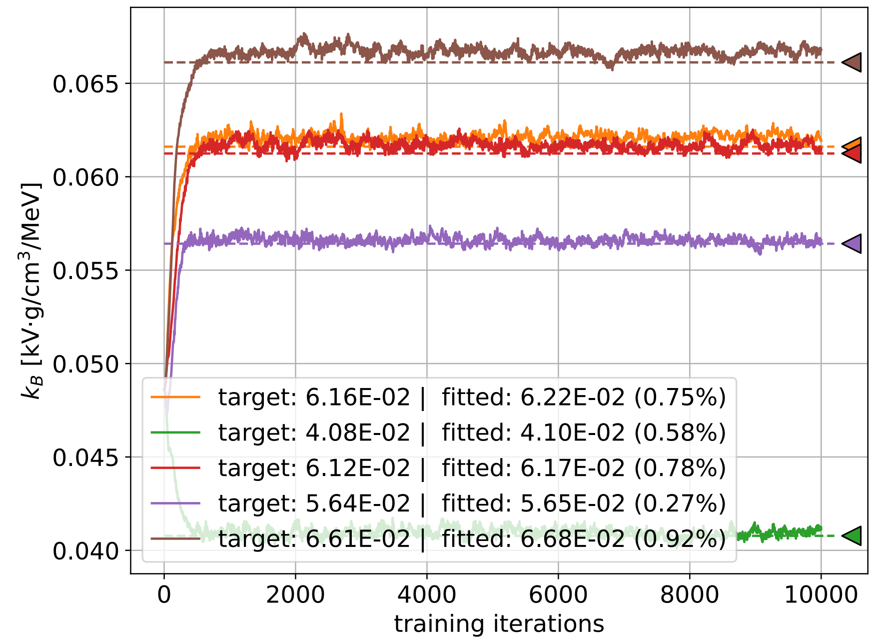
Calibration Test with Reconstructed dE/dx

$\mathcal{L}(f(\chi, \theta), f(\chi', \theta_{\text{target}}))$ **5 fits with different targets in the 6D phase space**

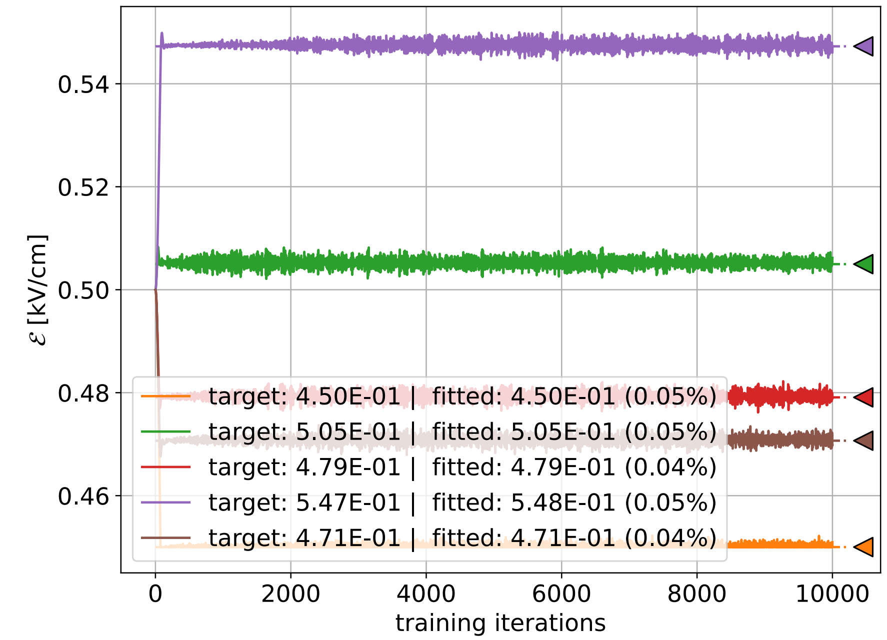
Recombination model A_B



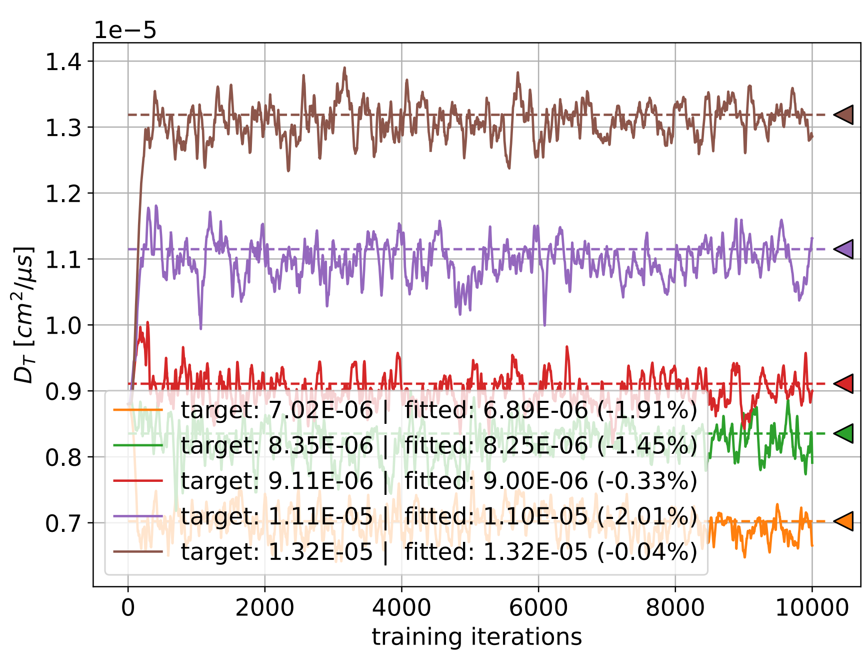
Recombination model k_B



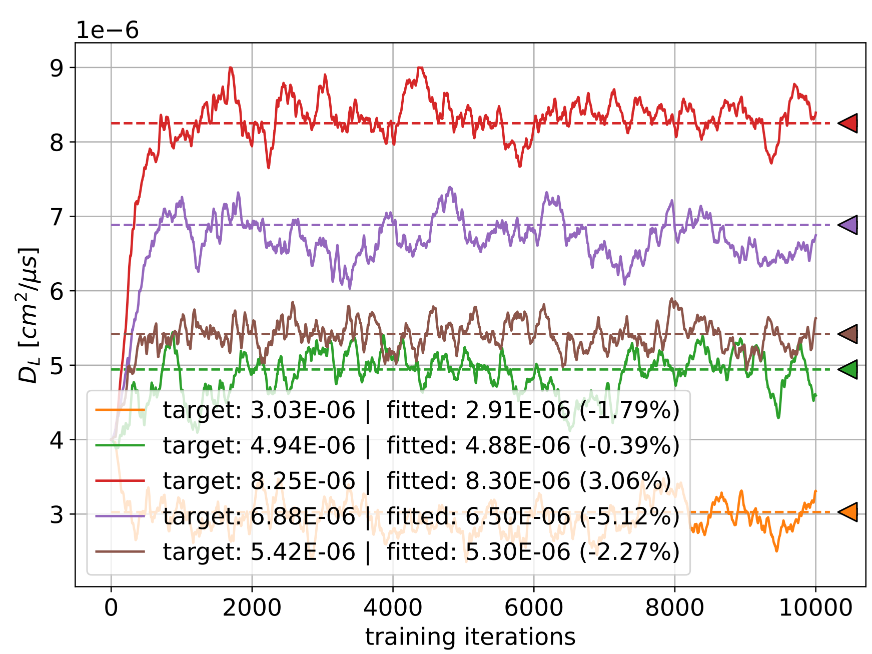
Electric field



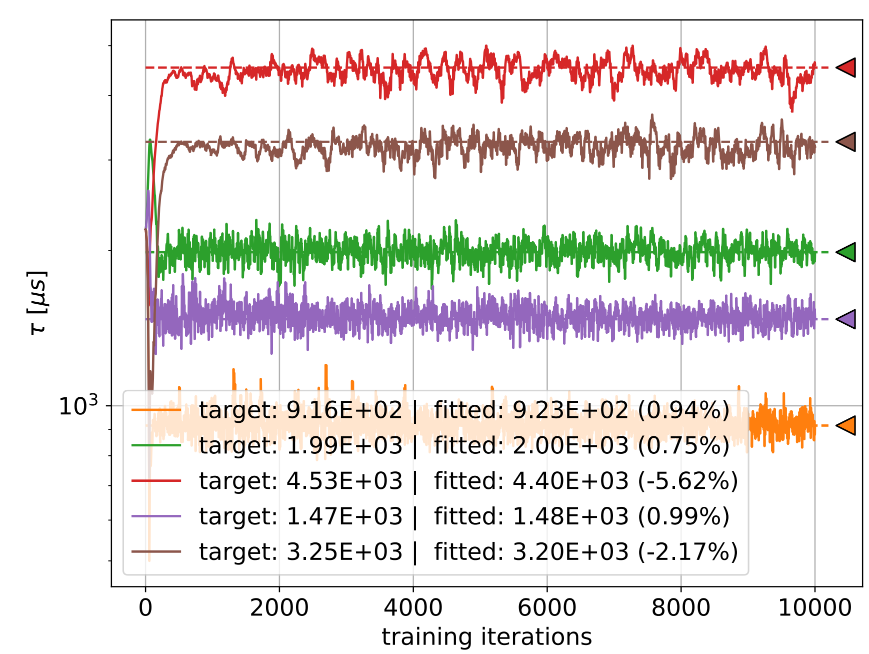
Transverse diffusion coefficient



Longitudinal diffusion coefficient



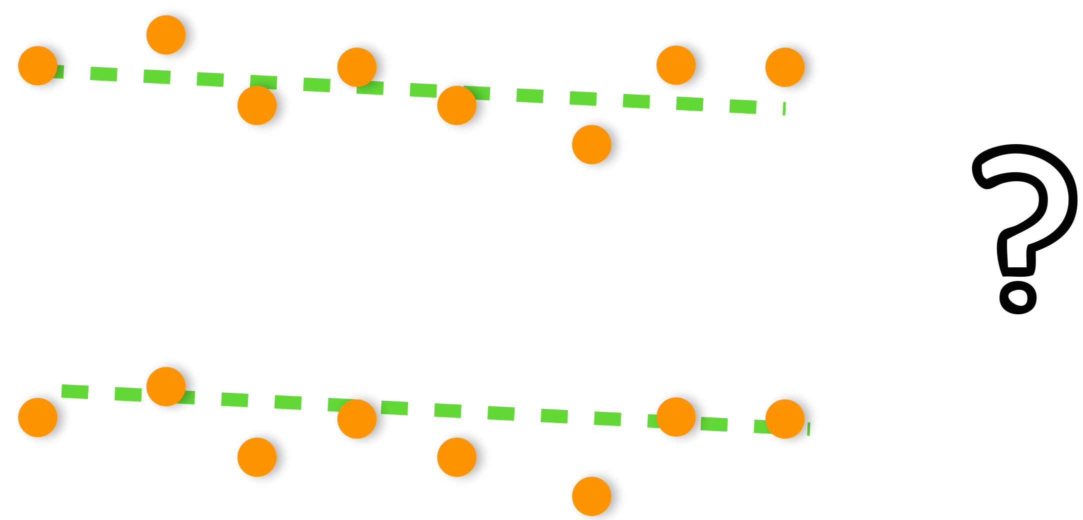
Electron lifetime



Reconstruct Simulation Input—Positional Shifts

$$\mathcal{L}(f(\underline{\chi}, \theta), \underline{F_{\text{target}}})$$

dE/dx, $\boxed{\text{x, y, z}}$

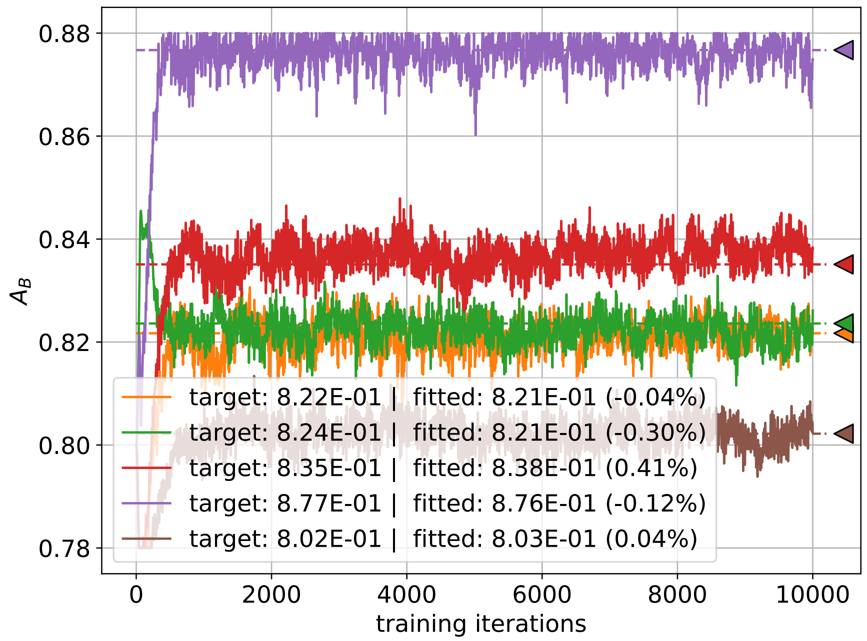


Possible positional shifts arise from input reconstruction

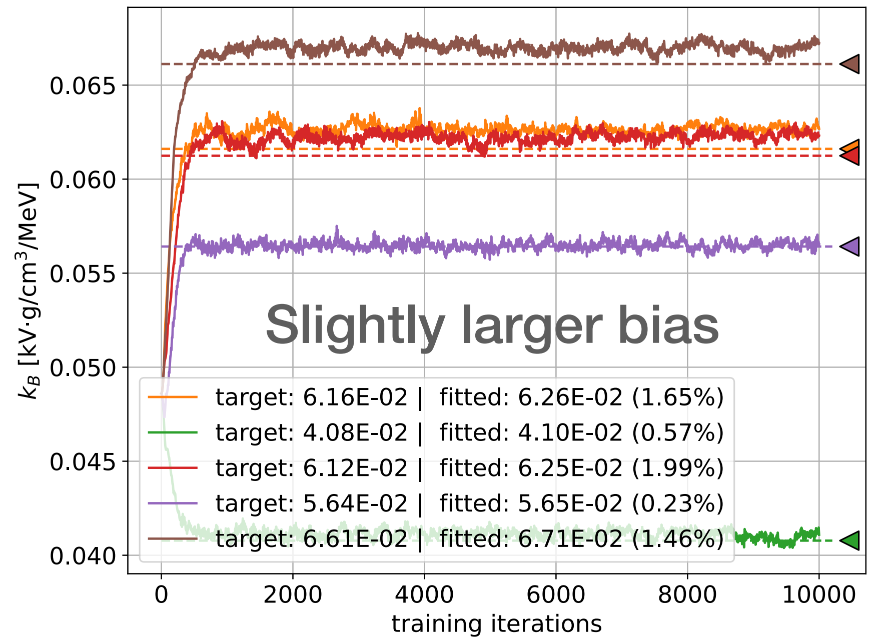
Robustness Test with Shifted Drift (0, 0.3) cm

$\mathcal{L}(f(\underline{\chi}, \theta), f(\underline{\chi'}, \theta_{\text{target}}))$ **5 fits with different targets in the 6D phase space**

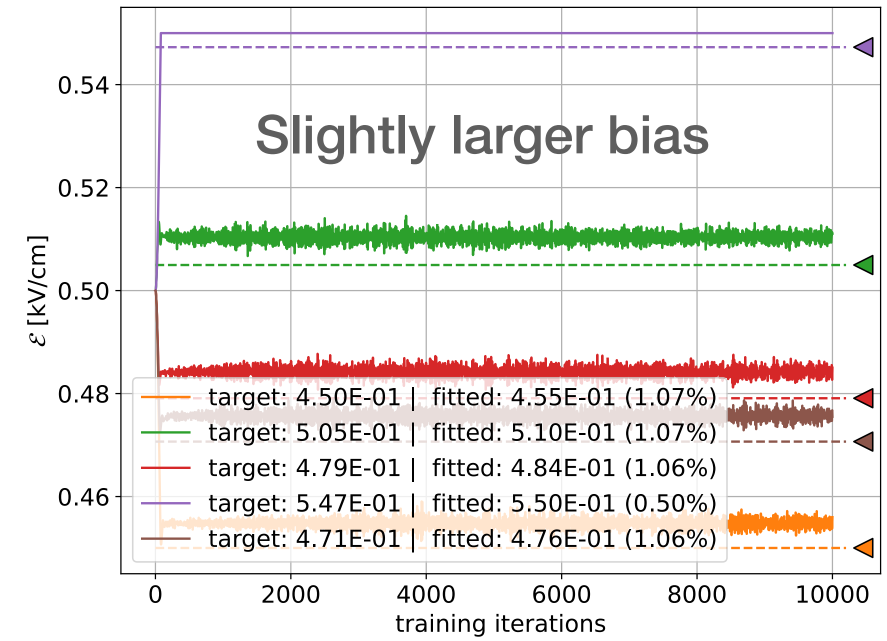
Recombination model A_B



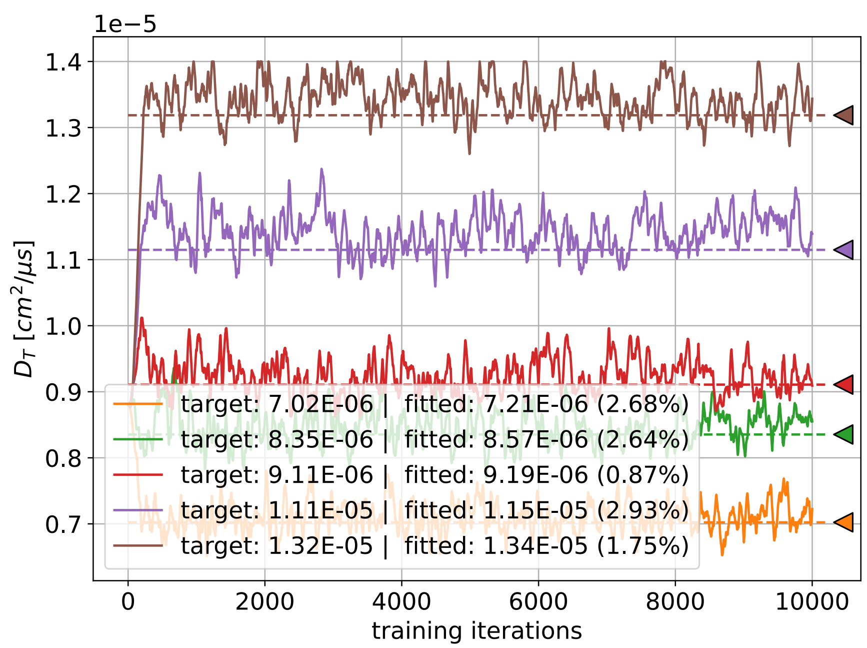
Recombination model k_B



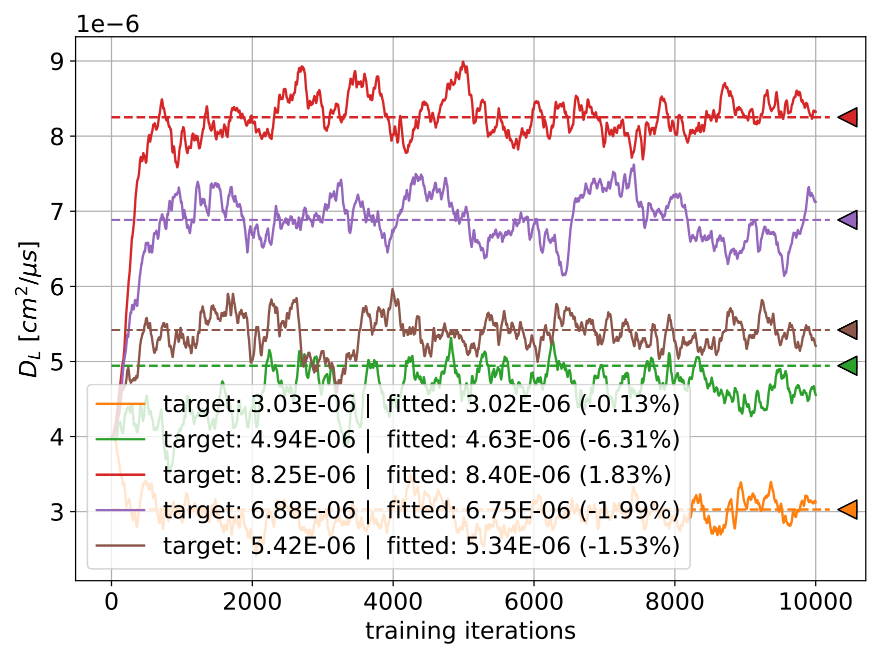
Electric field



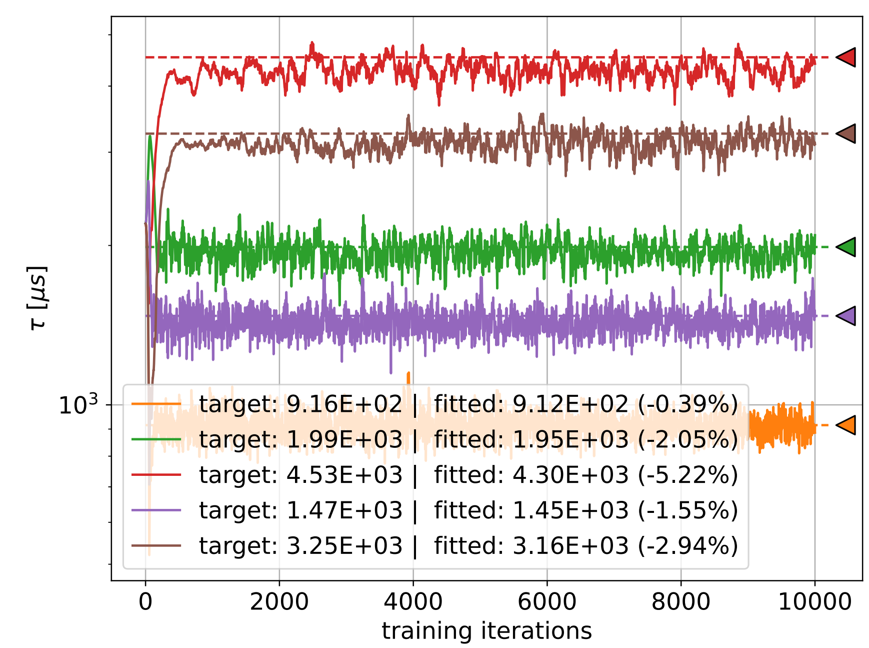
Transverse diffusion coefficient



Longitudinal diffusion coefficient



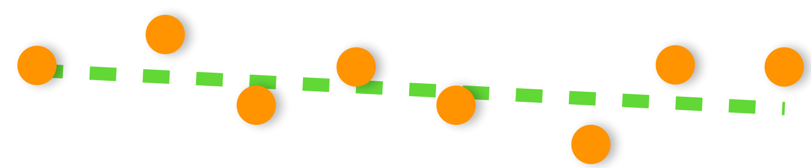
Electron lifetime



Reconstruct Simulation Input—Impurities

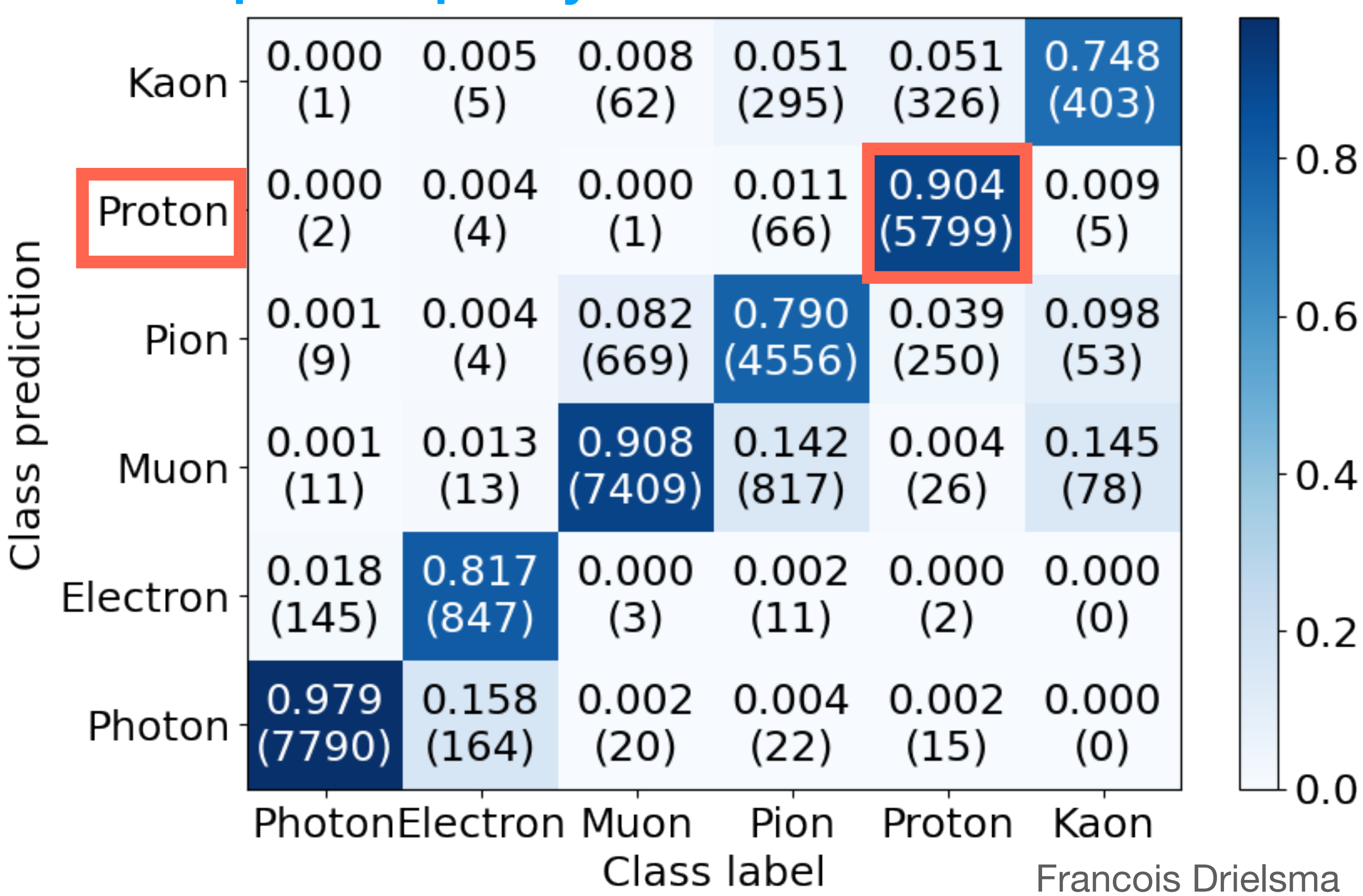
$$\mathcal{L}(f(\chi, \theta), F_{\text{target}})$$

dE/dx x, y, z

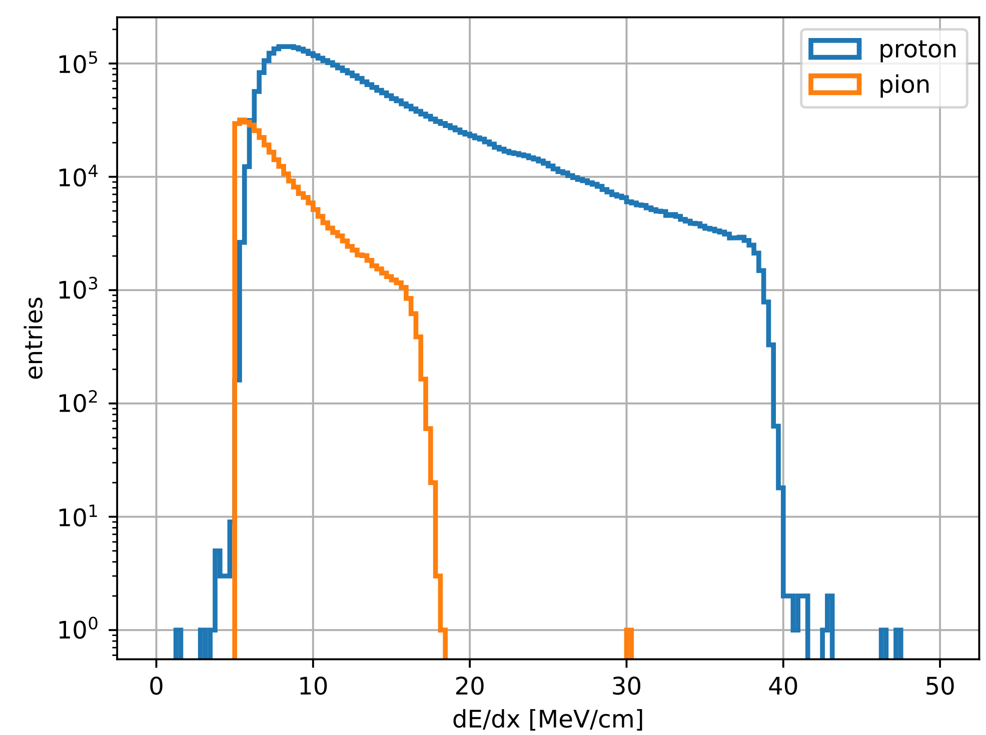


Stopping protons Stopping muons

SPINE
98% proton purity



90% protons, 10% pions

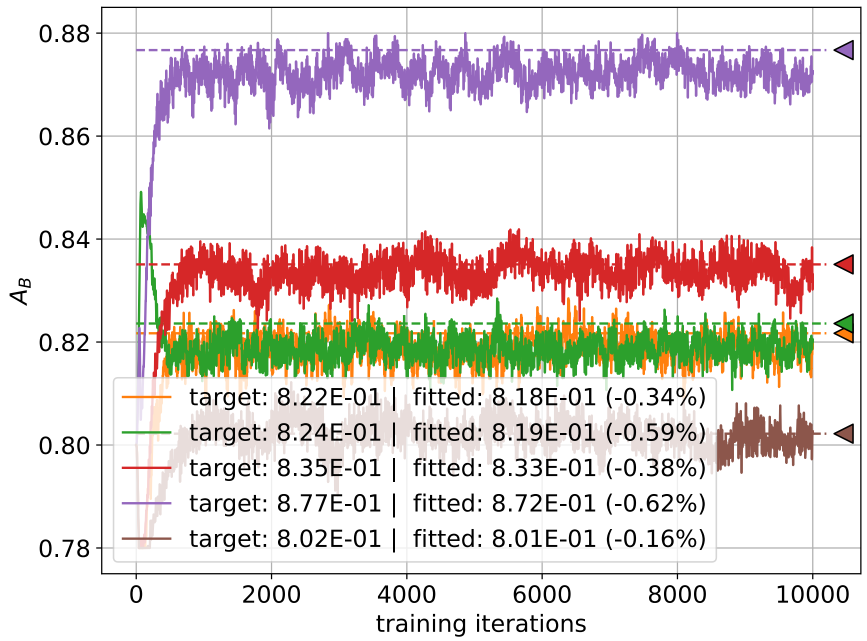


Francois Drielsma

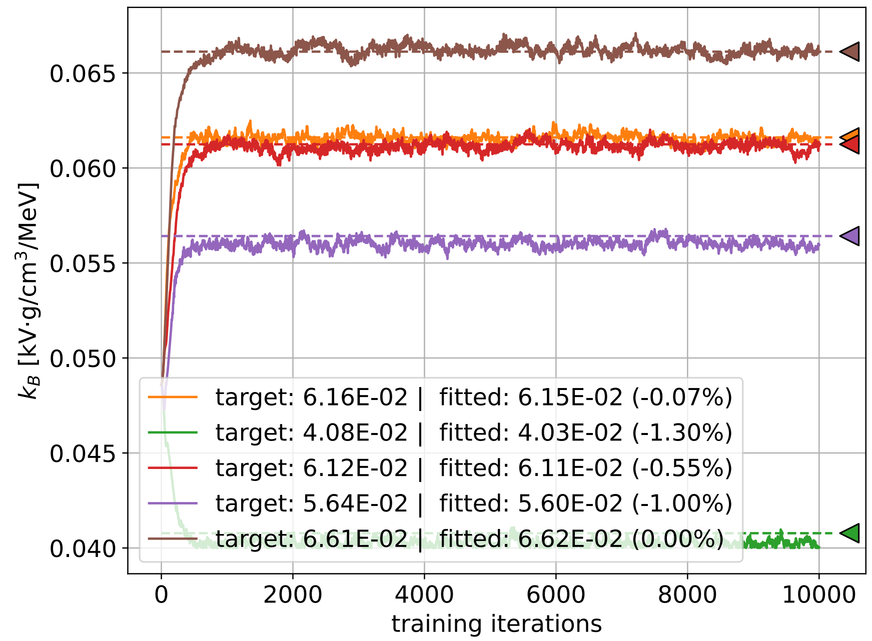
Robustness Test with 10% Mixed Pions

$\mathcal{L}(f(\underline{\chi}, \theta), f(\underline{\chi'}, \theta_{\text{target}}))$ **5 fits with different targets in the 6D phase space**

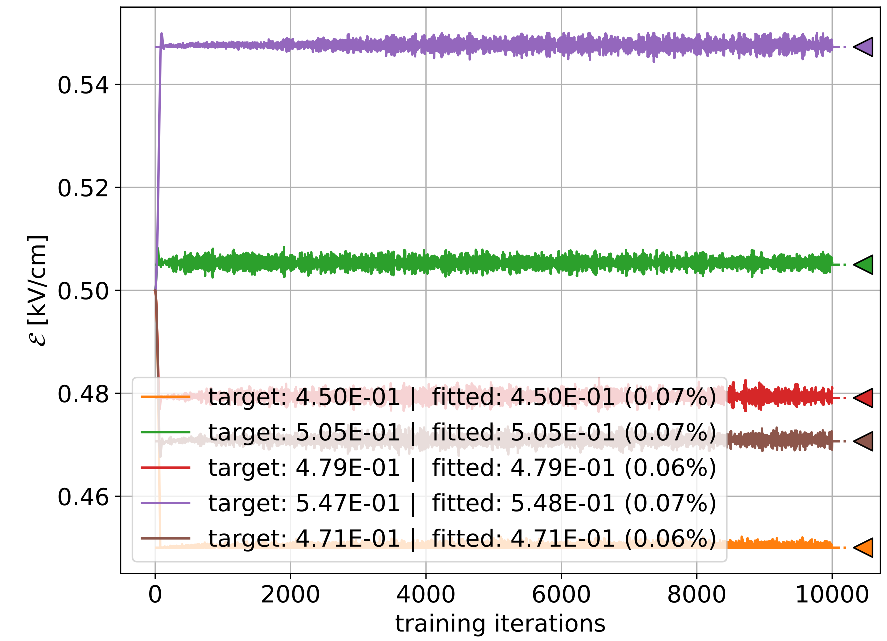
Recombination model A_B



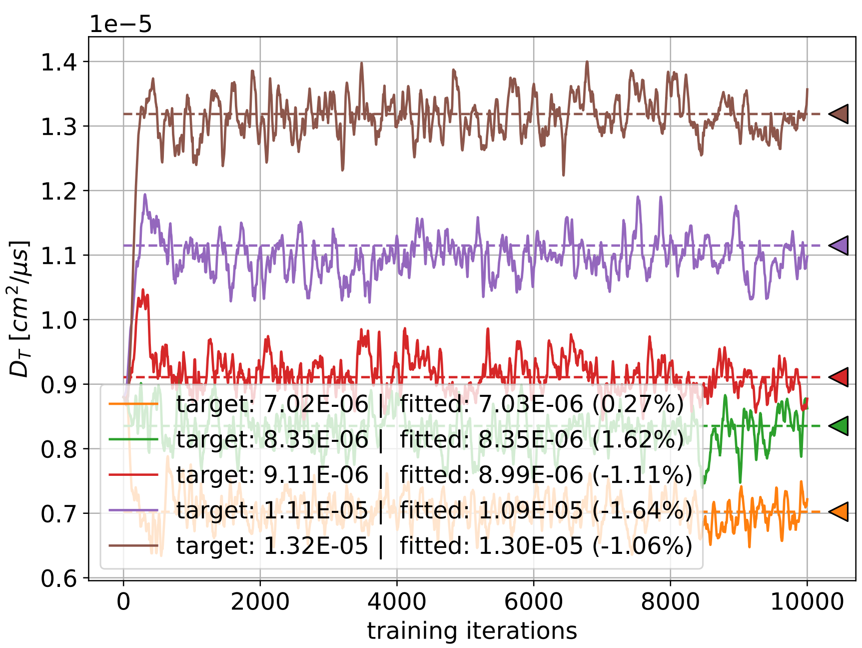
Recombination model k_B



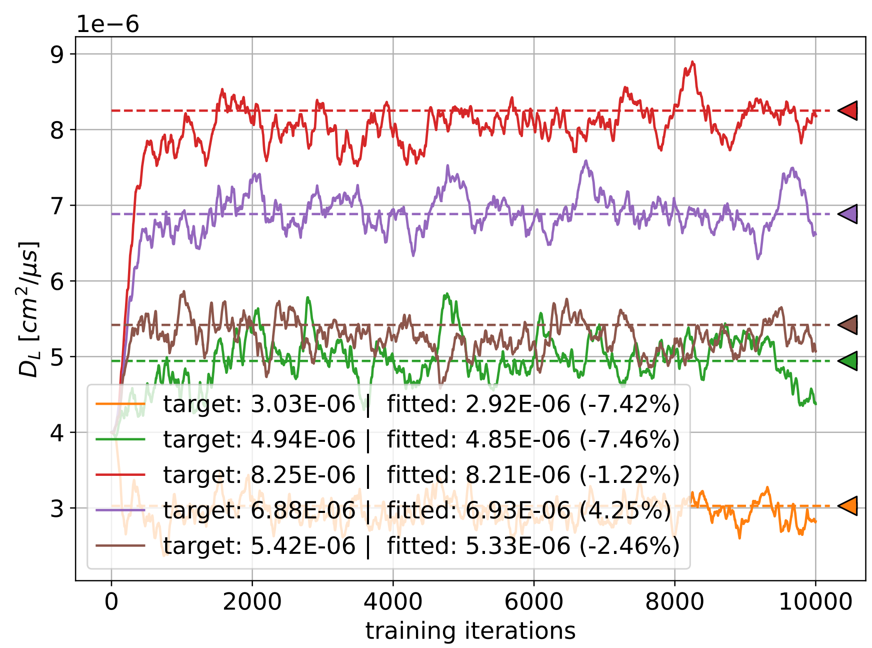
Electric field



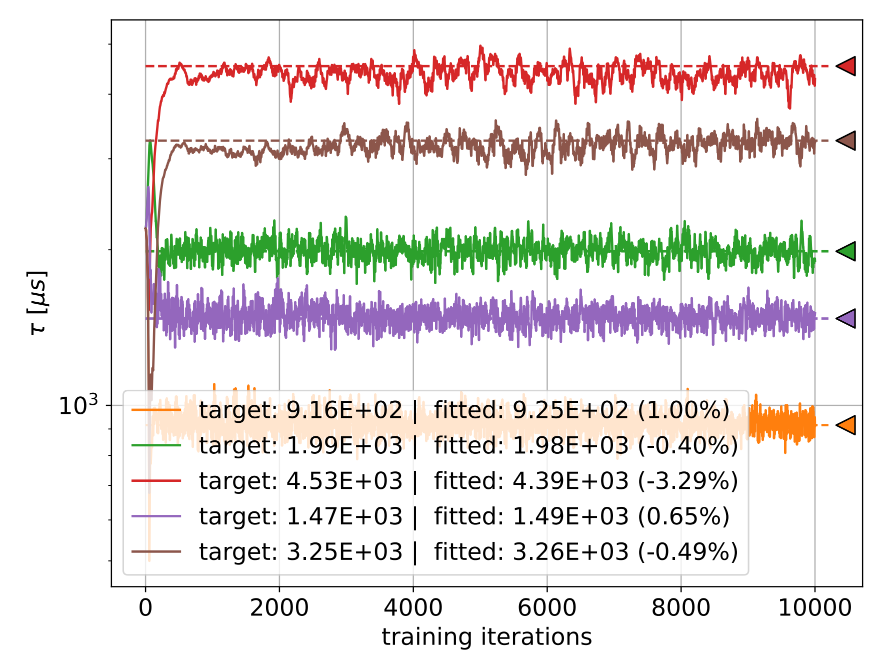
Transverse diffusion coefficient



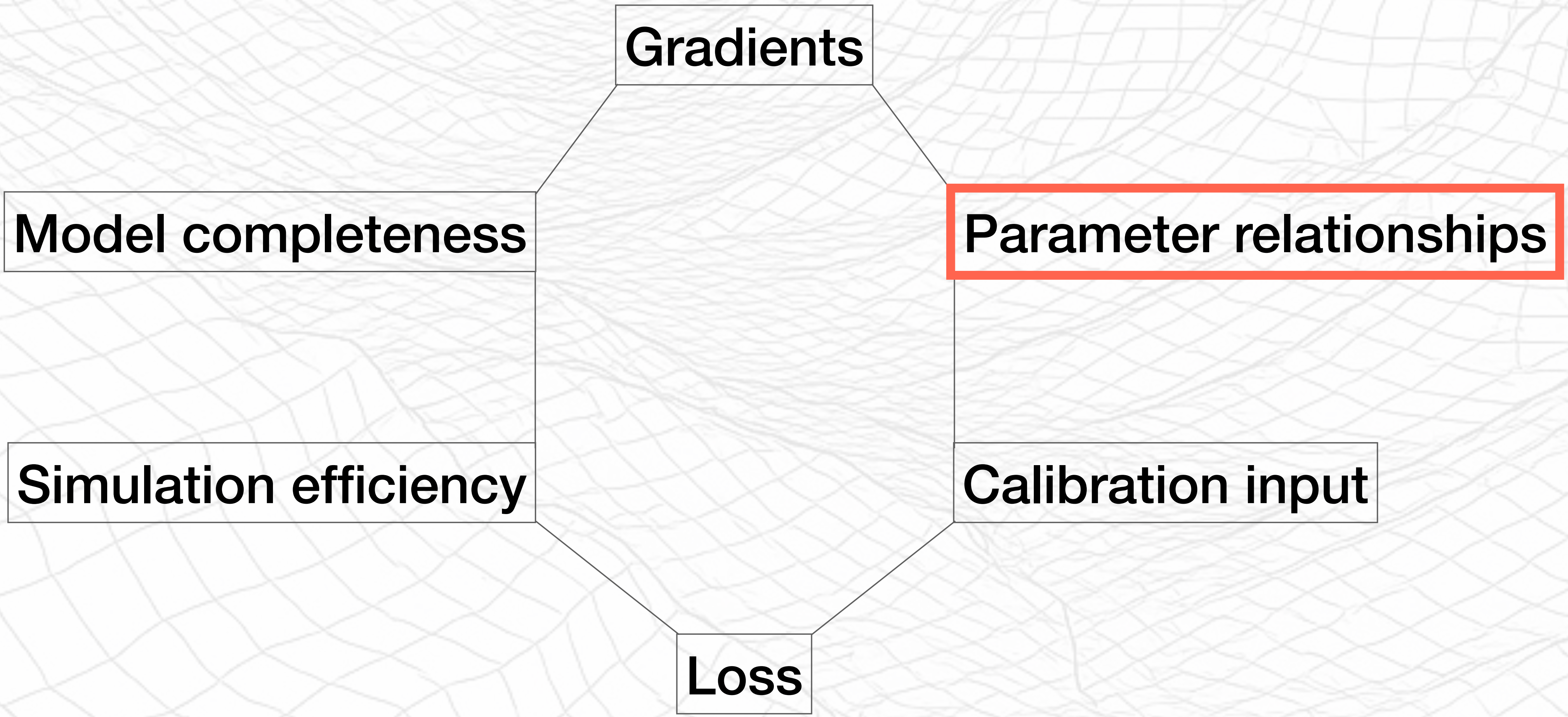
Longitudinal diffusion coefficient



Electron lifetime



Roadmap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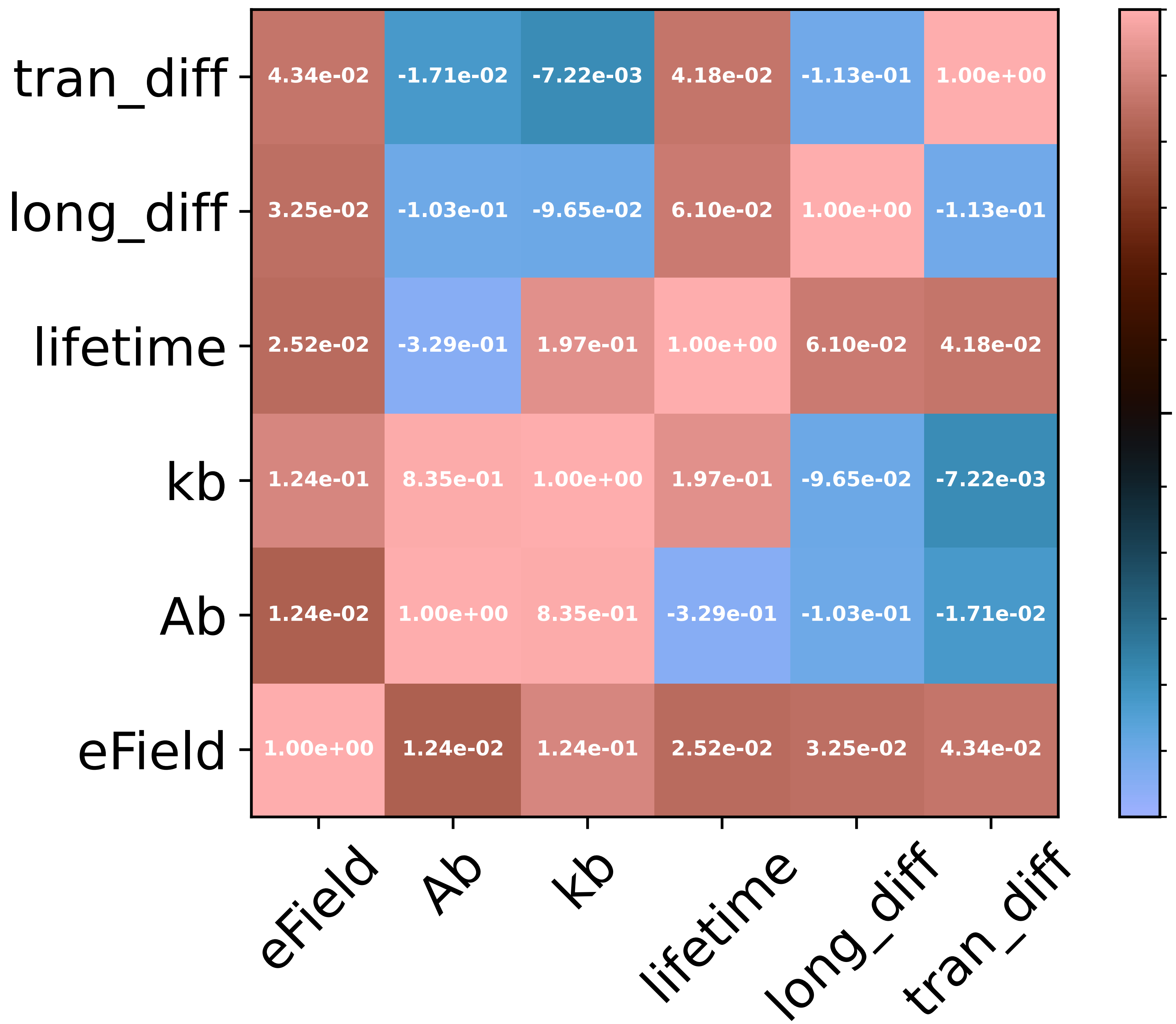
Pseudo-Correlation

Calculate Hessian from 1000 batches of 200 cm tracks
Normalized Hessian shows curvatures of the loss wrt. the parameters
Pseudo-covariance and correlation with normalization and regularization



Calibration with Differentiable Simulation