# ML AND DIFFERENTIABLE PROGRAMMING OPTIMIZATION FOR X-RAY SPECTROSCOPY

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John Templeton Foundation

CENTRO FERMI MUSEO STORICO DELLA FISICA E CENTRO STUDI E RICERCHE ENRICO FERMI

FWF Der Wissenschaftsfonds.

TEQ

FQXi FOUNDATIONAL QUESTIONS INSTITUTE

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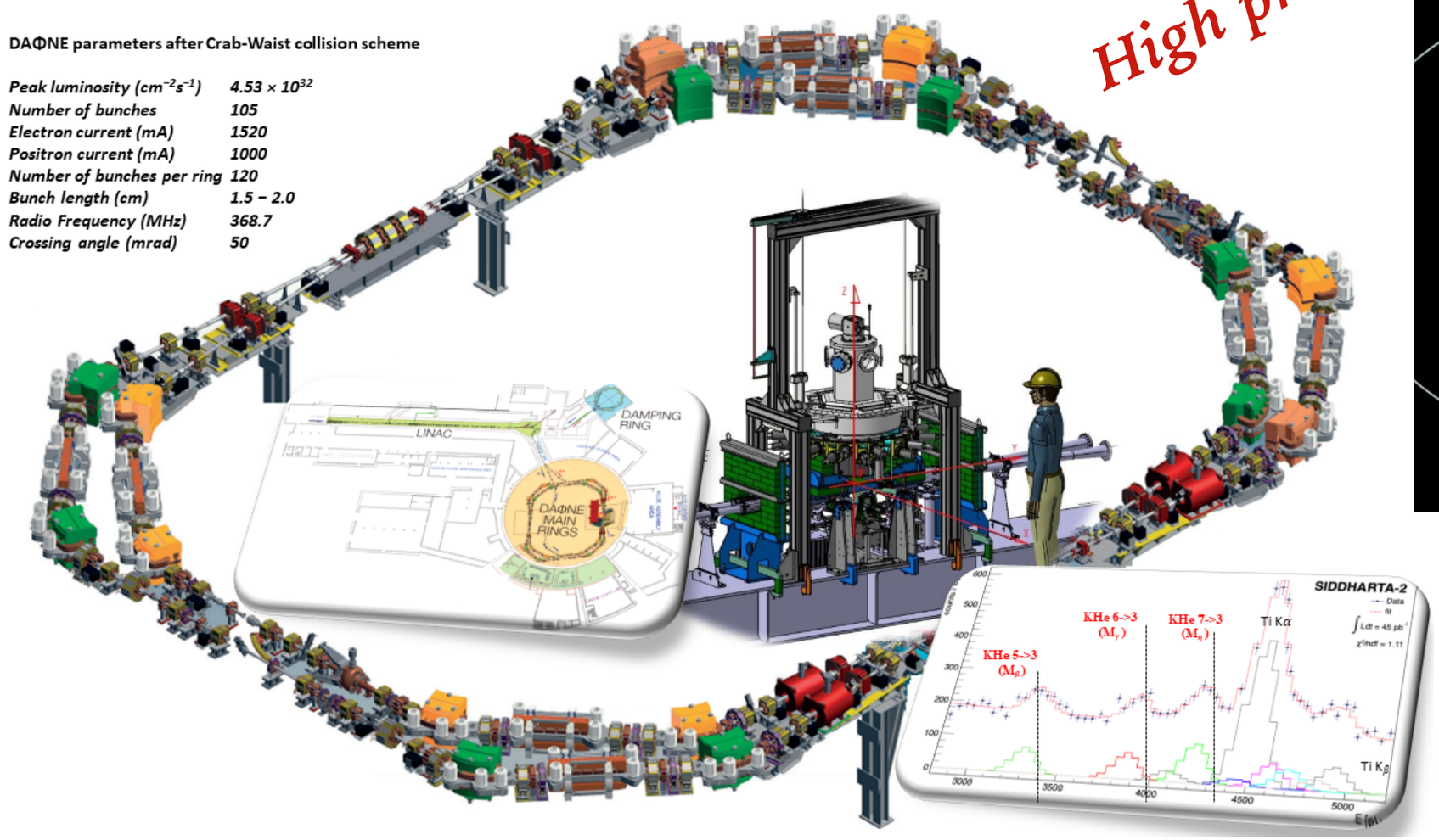
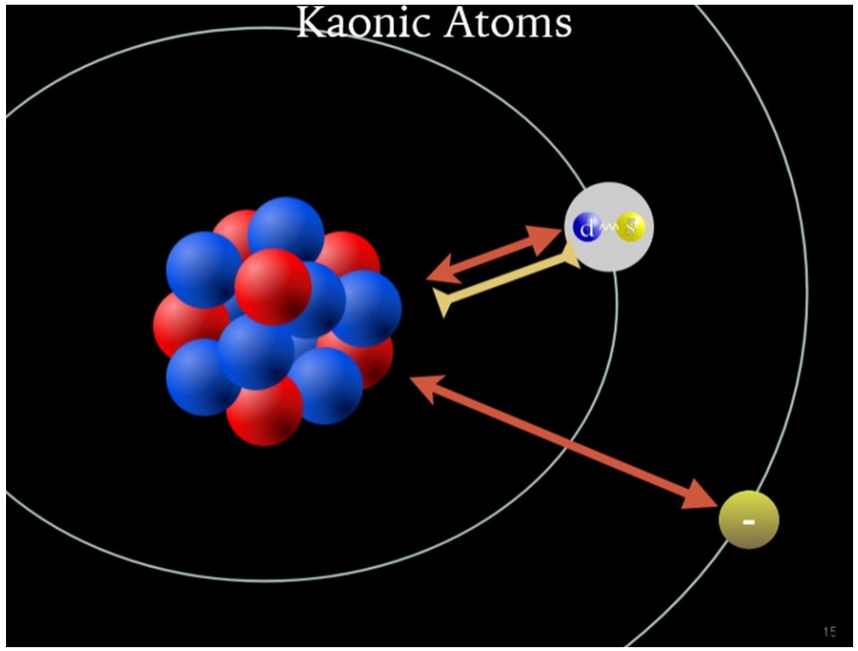
*ALPACA: modern algorithms in machine learning and data analysis: from medical physics to research with accelerators and in underground laboratories*

*ECT* Trento, 24/11/23*

# SIDDHARTA-2 experiment at INFN-LNF

**High precision needed!**



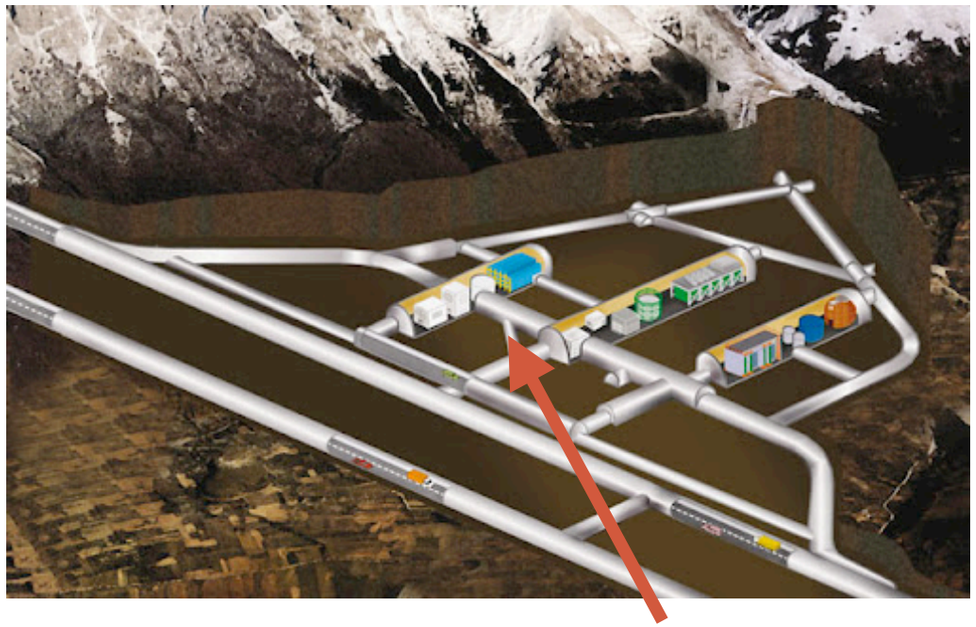




*See F. Sirghi & S. Manti talks on Tuesday*

*Precision x-ray spectroscopy of exotic systems*

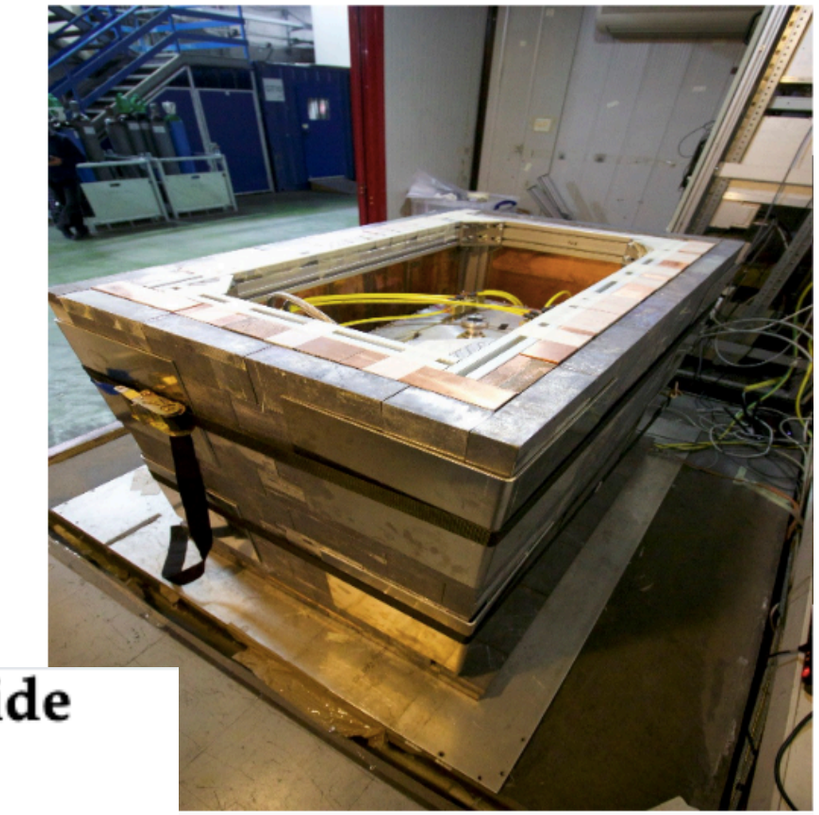
- *extract low-energy observables in strangeness sector*
  - *Implications to many areas: astrophysics, neutron stars EoS, dark matter, nuclear & fundamental physics*

# *VIP-2 experiment at INFN-LNGS*

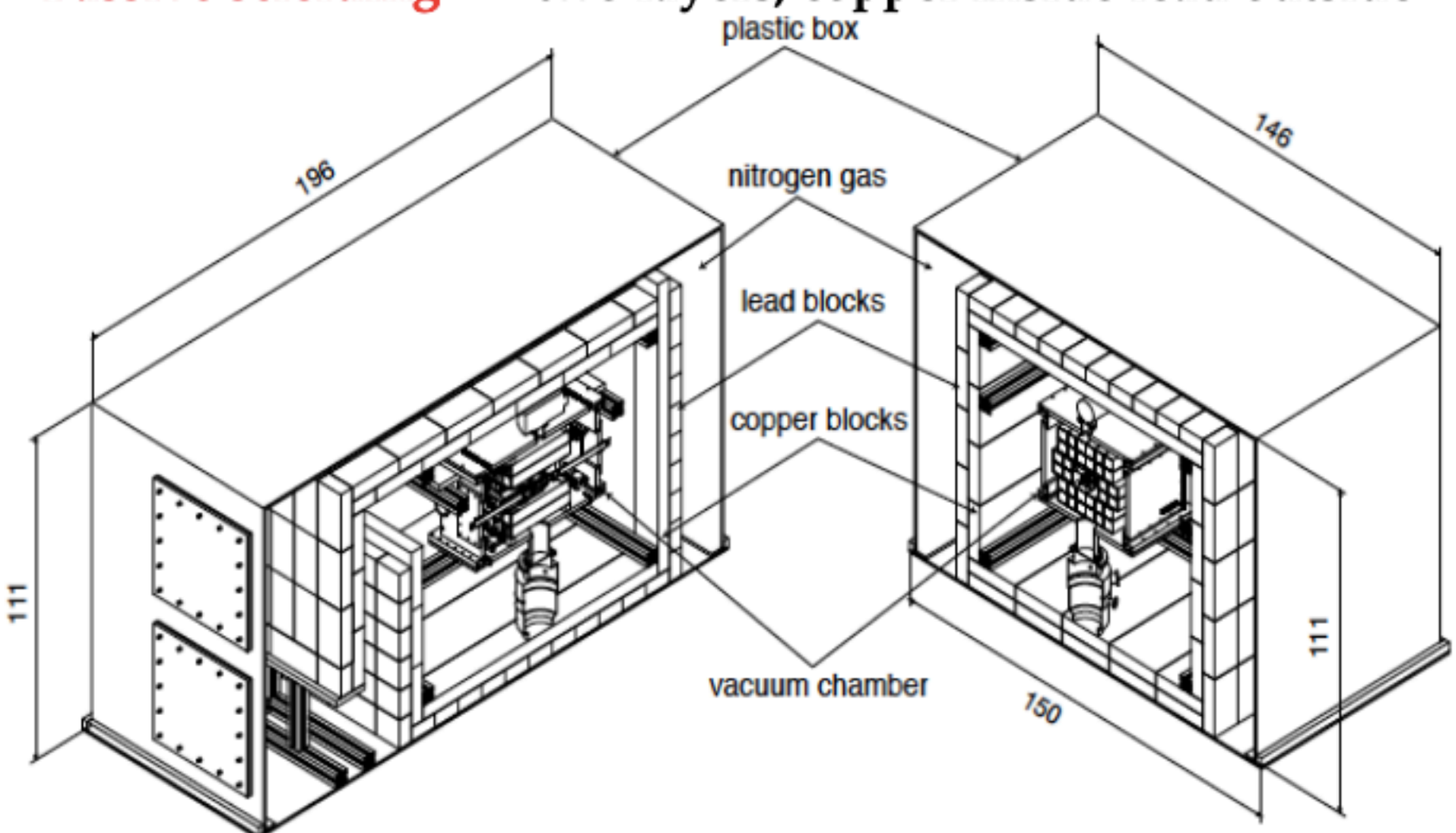


*1400 m rock coverage*

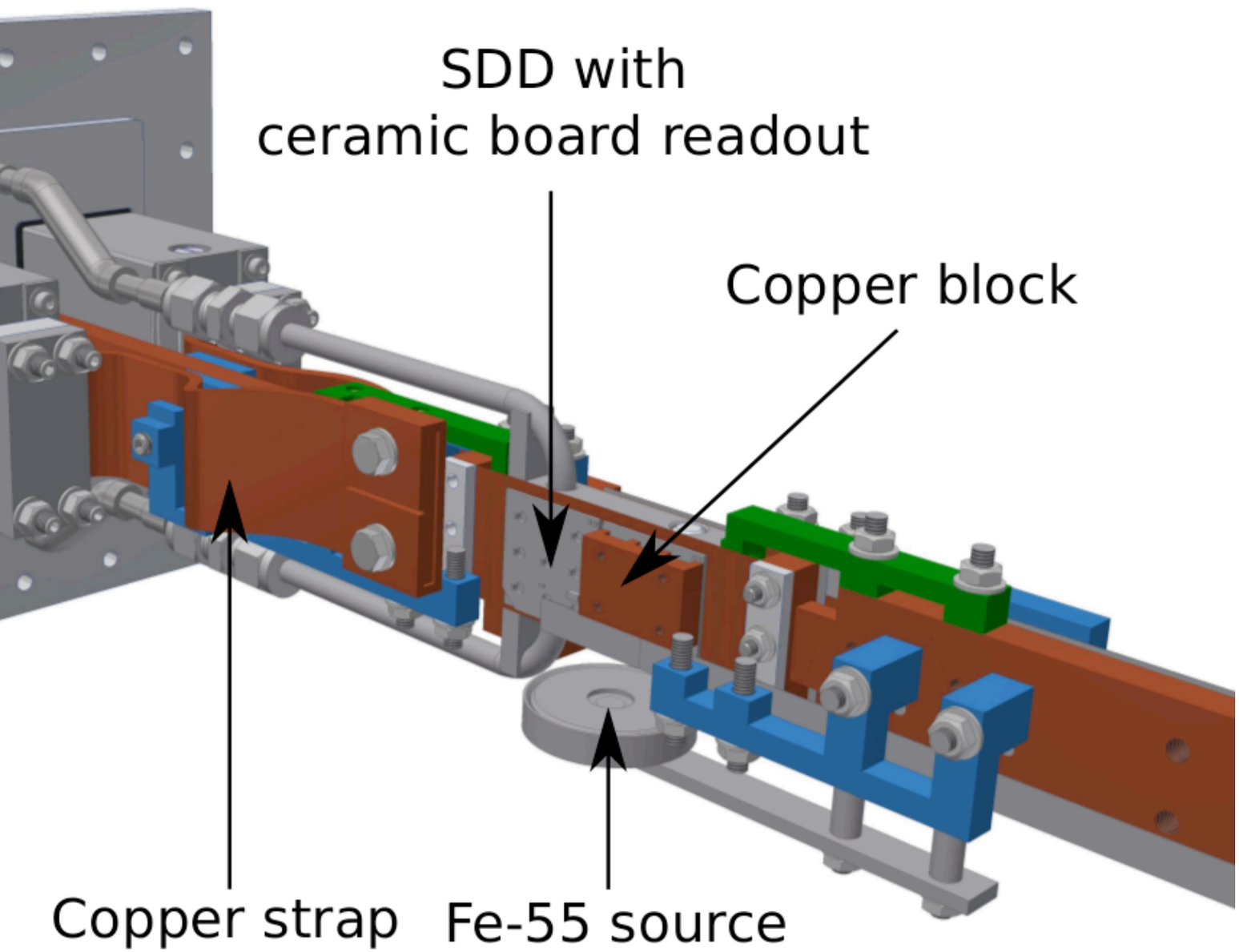
**Upgrade concluded in April 2019:**



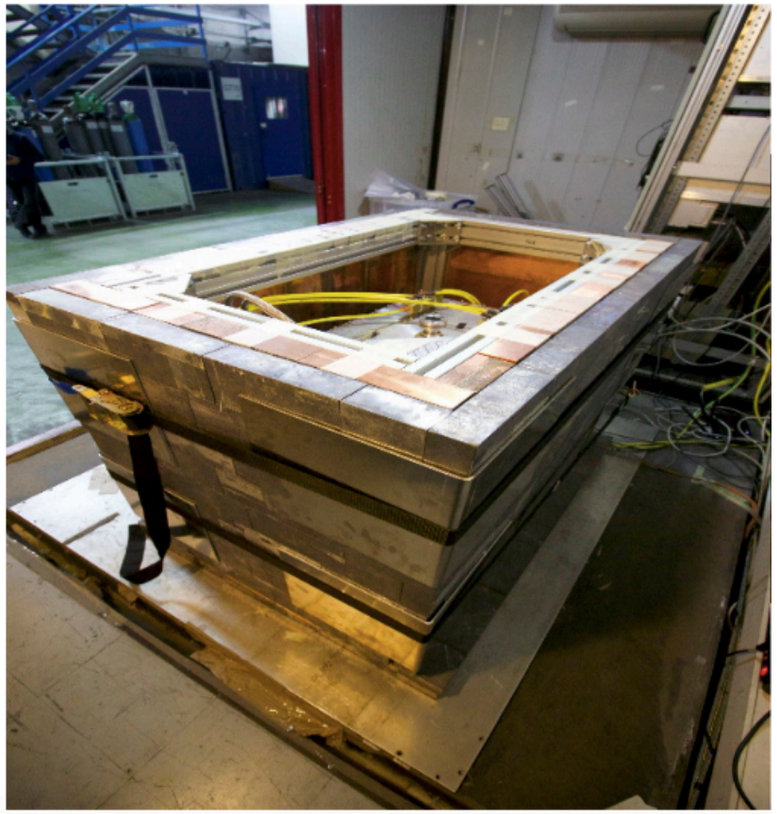
**Passive scielding → two layers, copper inside lead outside**



# VIP-2 experiment at INFN-LNGS



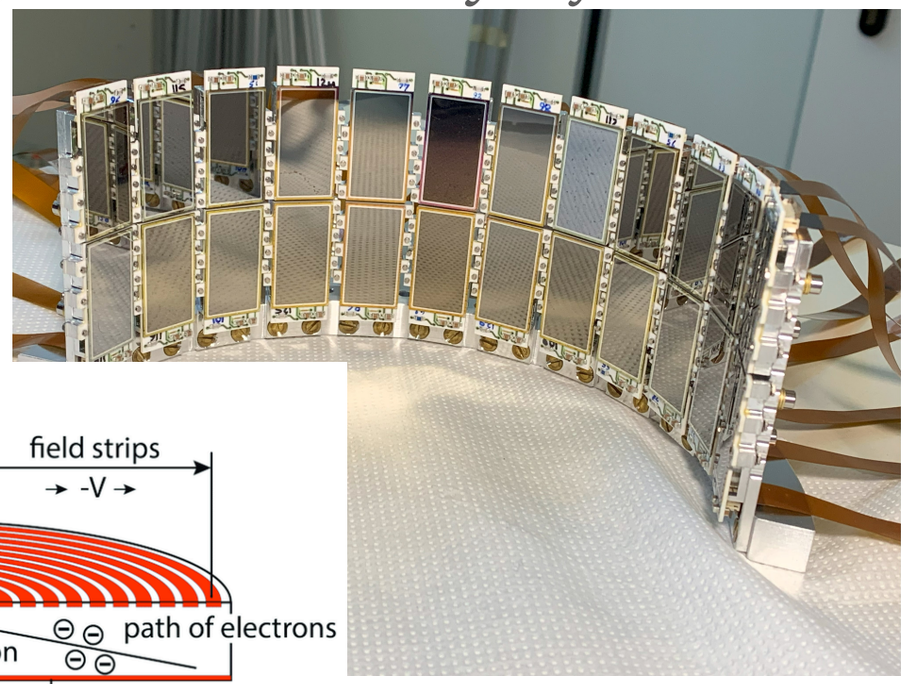

**Upgrade concluded in April 2019:**

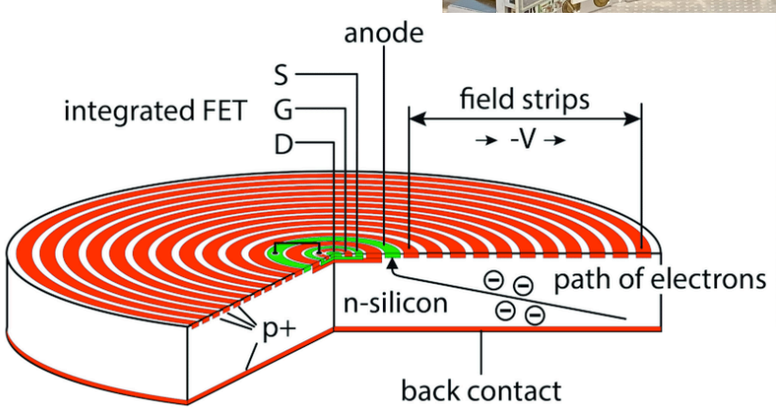


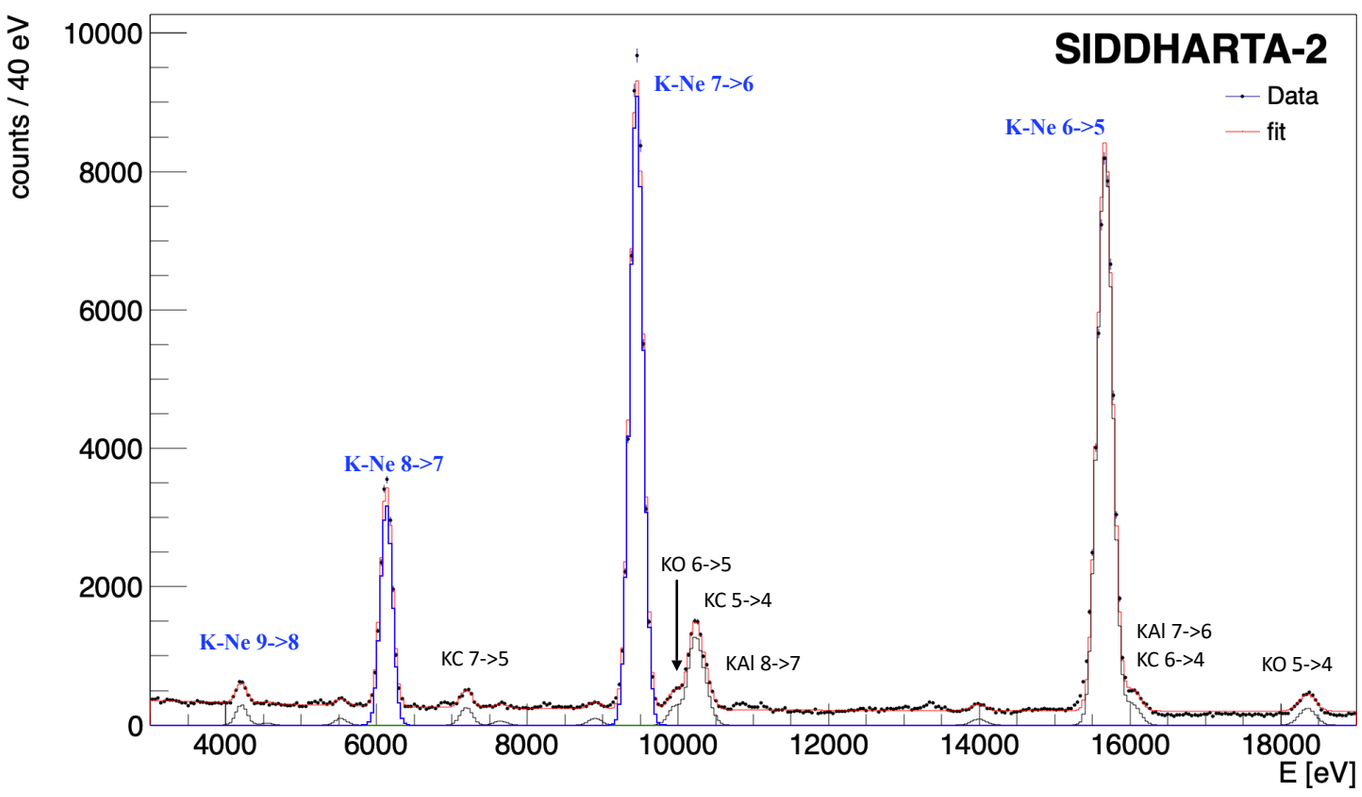
*Searching for Pauli Exclusion Principle Violations*

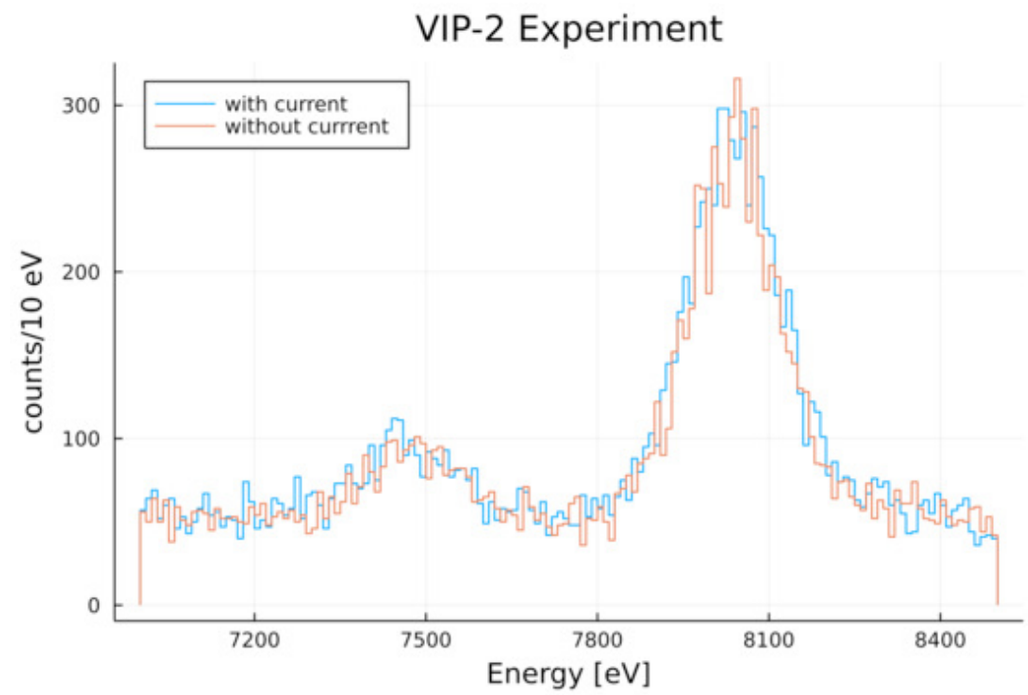
*Quantum Gravity*

*Silicon Drift Detectors (**SDDs**) high (190 eV FWHM at 8.0 →keV), faster (triggerable) detectors. Arrays of 2 x 4 SDDs 8mm x 8mm each, 450 um thick*



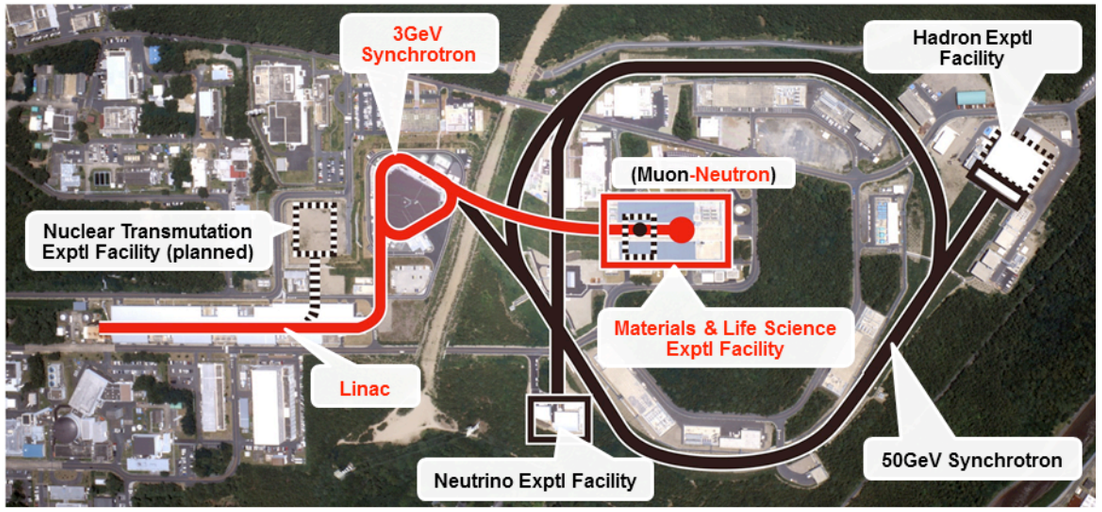


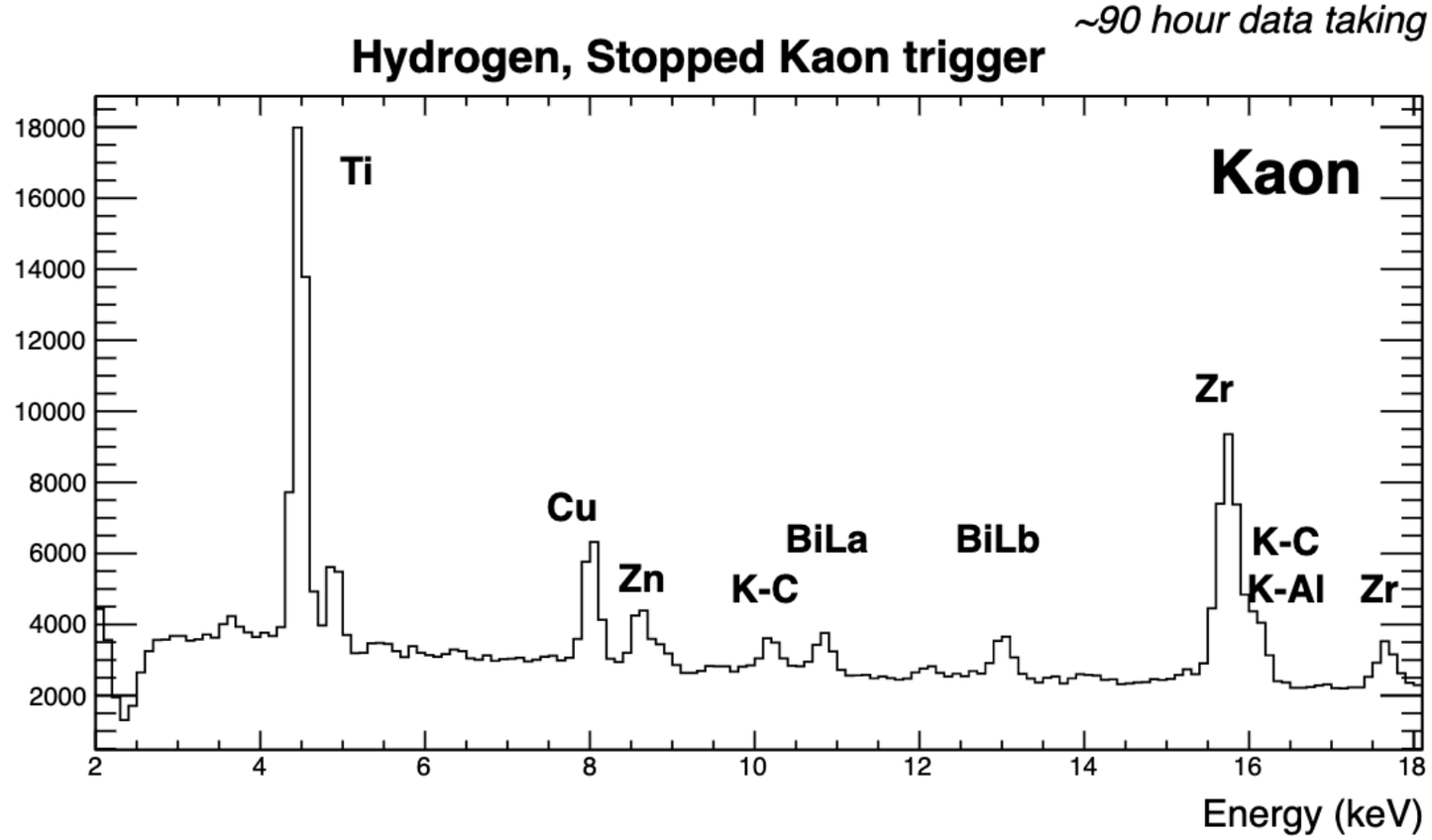

*Ideal tool for precision X-ray spectroscopy*

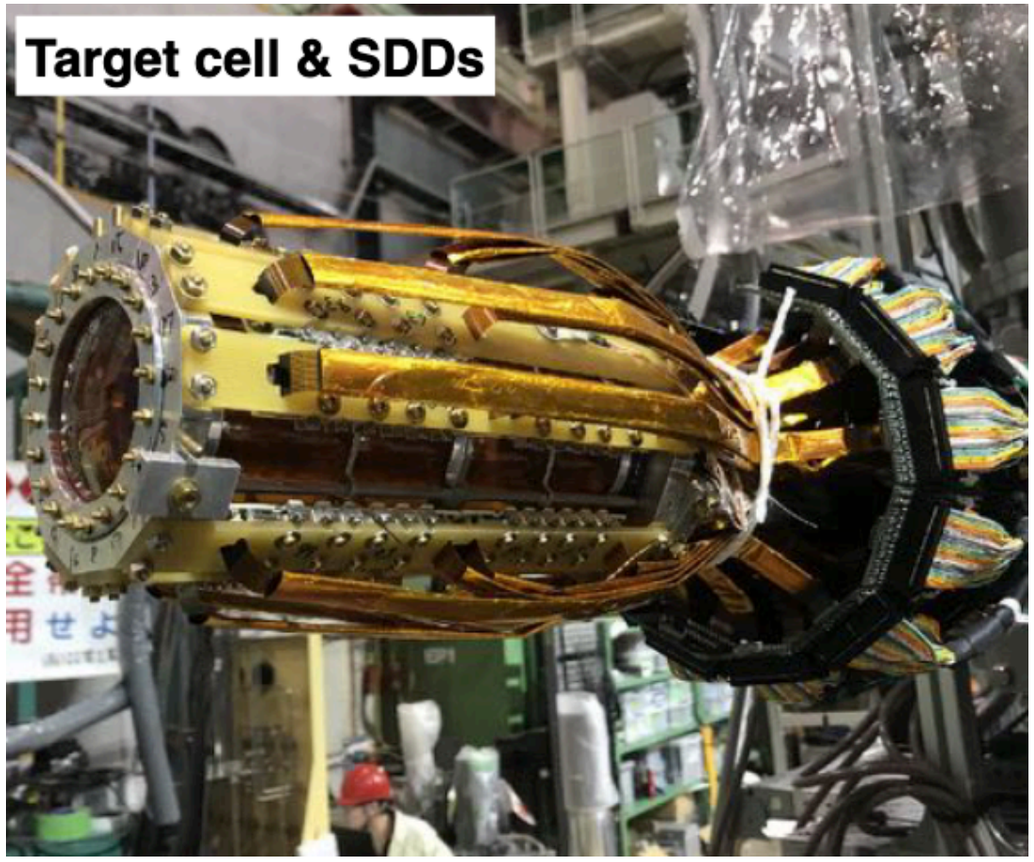
# More examples: kaonic atoms experiments at J-PARC




## Hydrogen data in E57

*~90 hour data taking*



# *Machine Learning in physics experiment*

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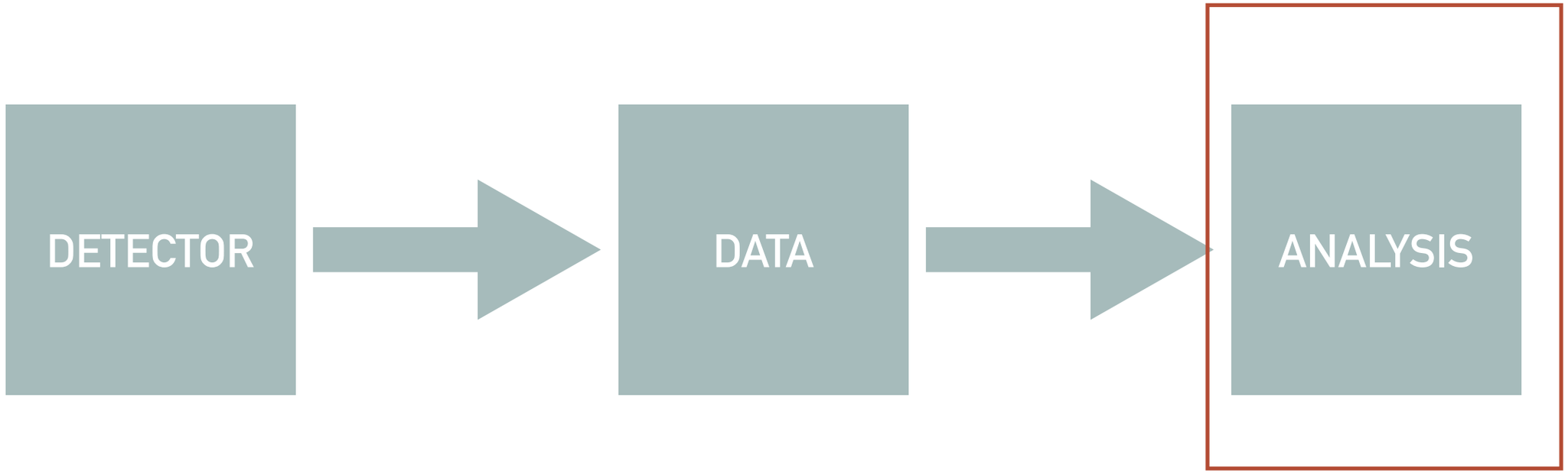
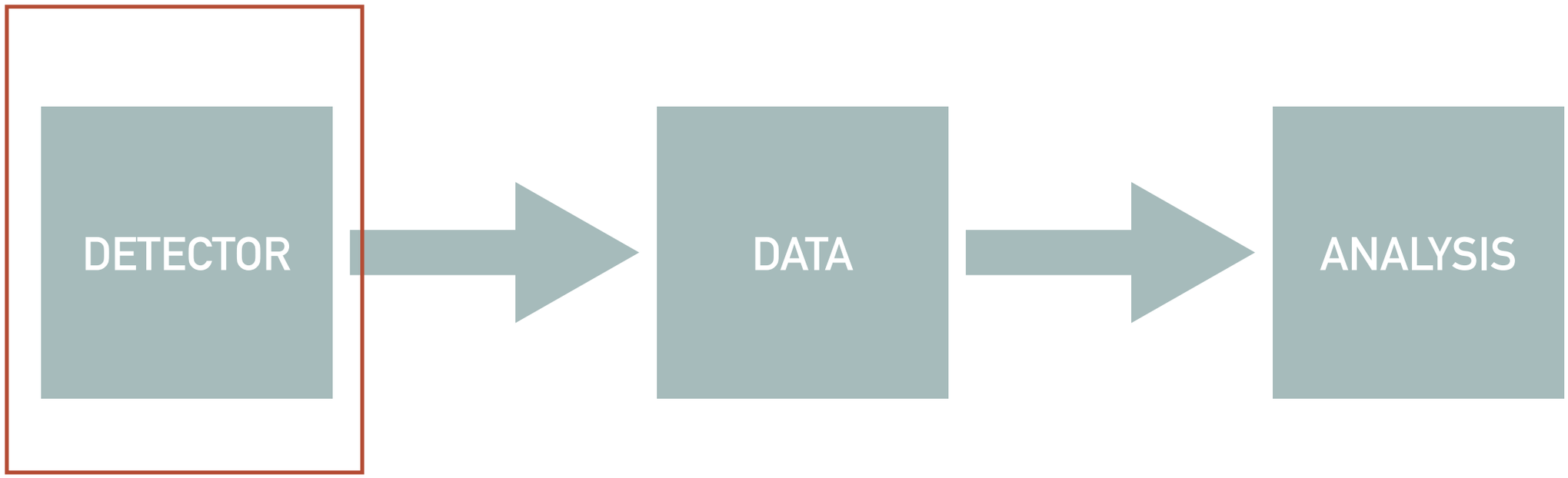



*ML improving the analysis:*
*S vs B classification,*
*object reconstruction,*
*data simulation*
*etc*

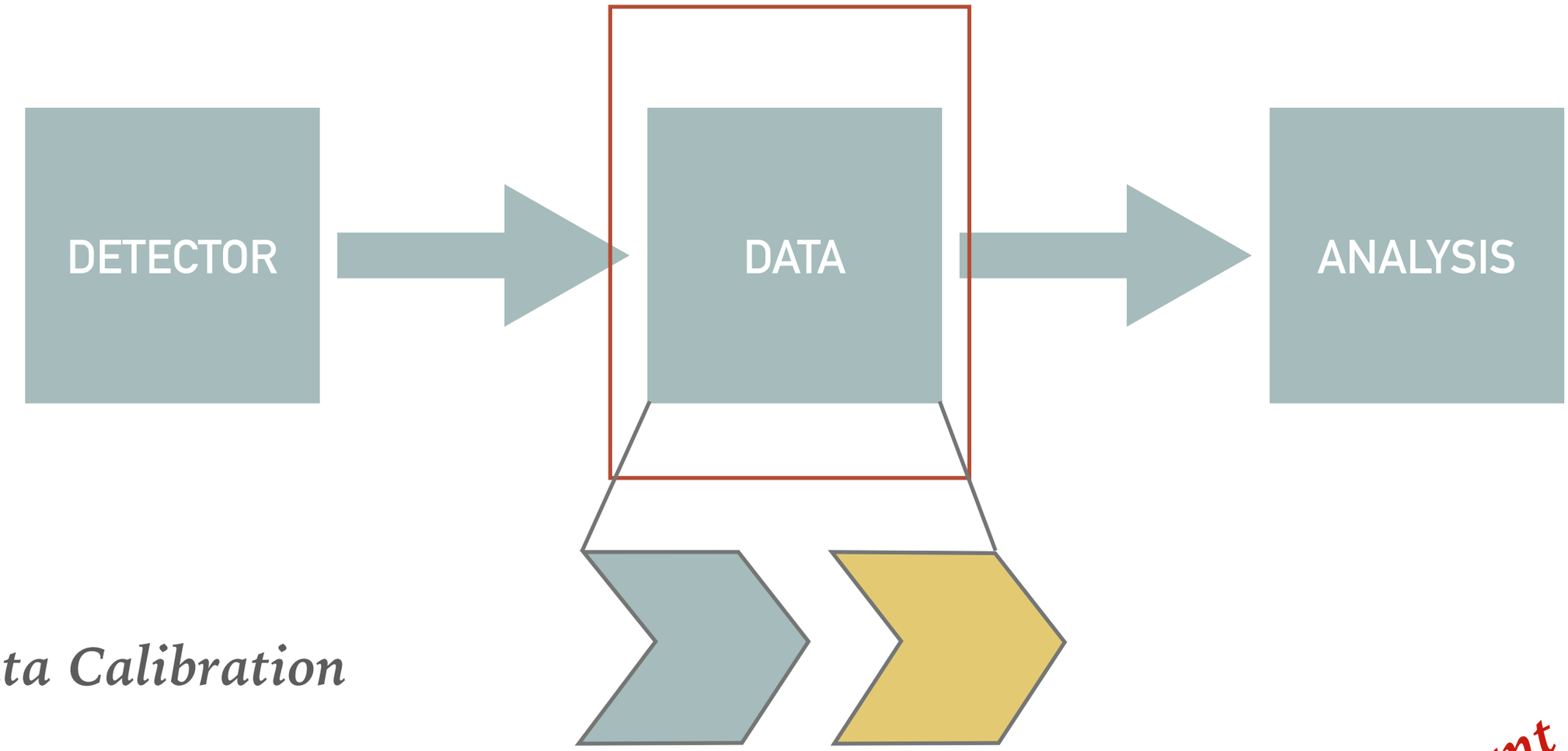
# *Machine Learning in physics experiment*




*e.g. optimization of detector geometry*

*See talks from Tommaso Dorigo & Pietro Vischia*

# Machine Learning in physics experiment




Data Calibration

Raw data

Calibrated data

Extremely important in x-ray spectroscopy

https://www.sciencedirect.com/science/article/pii/S0370269311001225

Using the correction term $\varepsilon$ in Eq. (2), the absolute energy of the kaonic $^3$He $3d \to 2p$ transition was then determined to be:

$$E_{\text{exp}} = E_{\text{fit}} + \varepsilon = 6223.0 \pm 2.4(\text{stat}) \pm 3.5(\text{syst})\text{eV}, \quad (4)$$

where the second term is the statistical error, and the third term is the systematic error. The latter was evaluated from the accuracy of the energy determination (±3.5 eV). Other contributions to the systematic error (e.g. effects of timing region selection and contributions of the kaonic oxygen line at 6.0 keV) are negligible.

*Kaonic He-3/4 Measurement @ DAFNE*

As a result, the $1s$-level shift $\epsilon_{1s}$ and width $\Gamma_{1s}$ of kaonic hydrogen were determined by SIDDHARTA to be

$$\epsilon_{1s} = -283 \pm 36(\text{stat}) \pm 6(\text{syst})\ \text{eV} \quad \text{and}$$
$$\Gamma_{1s} = 541 \pm 89(\text{stat}) \pm 22(\text{syst})\ \text{eV},$$

*E62 J-PARC measurement*

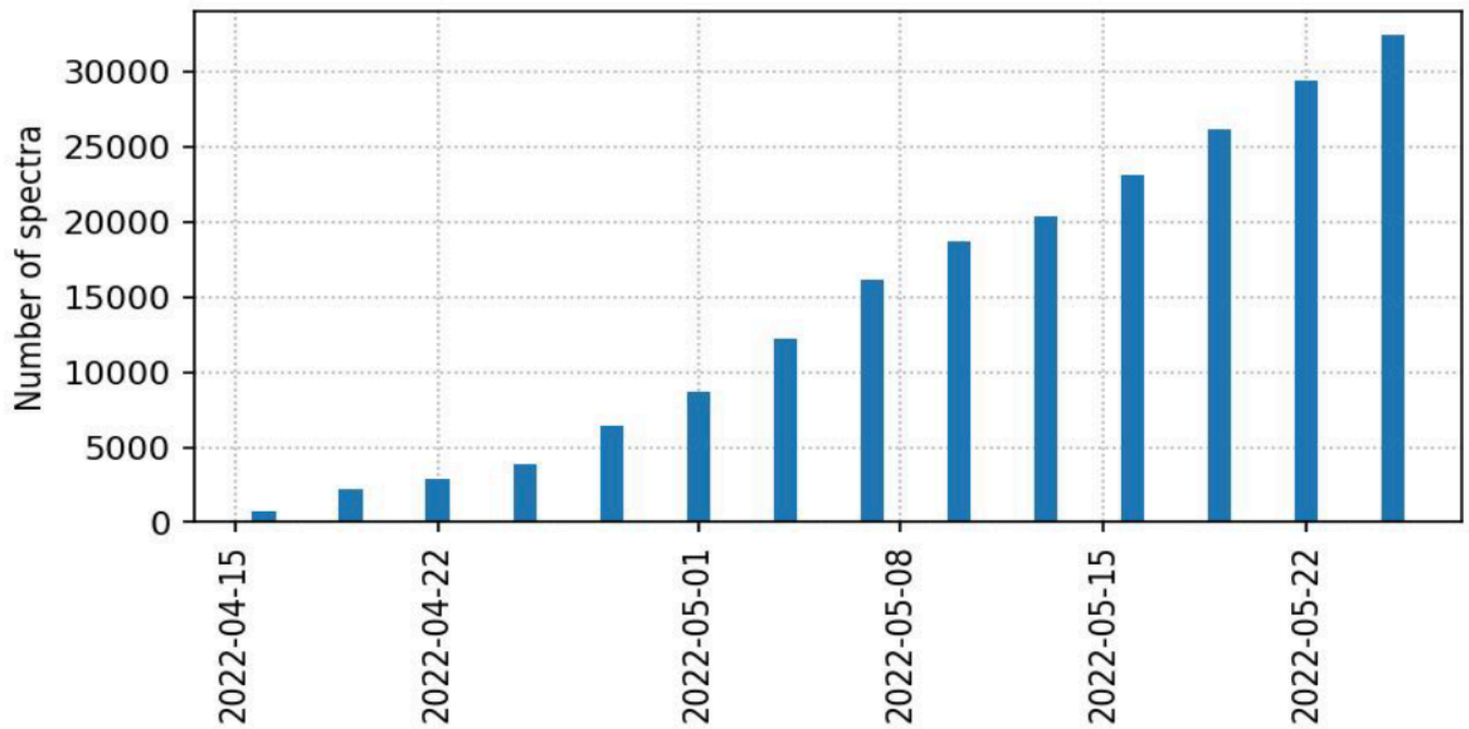
*PRL 128, 112503 (2022)*

TABLE I. Measured x-ray energies and widths of the kaonic $^3$He and $^4$He $3d \to 2p$ transitions, together with the summary of the statistical and systematic errors. Electromagnetic calculated energies are also tabulated. All the values are in units of eV.

| | $K^-{}^3$He | | $K^-{}^4$He | |
|---|---|---|---|---|
| | Energy | Width | Energy | Width |
| Measured ($E^{\text{exp}}_{3d\to 2p}$, $\Gamma_{2p}$) | 6224.48 | 2.5 | 6463.69 | 1.0 |
| Statistical error | 0.40 | 1.0 | 0.27 | 0.6 |
| Systematical error: total | 0.18 | 0.4 | 0.11 | 0.3 |
| (a) Absolute energy scale | 0.17 | ··· | 0.09 | ··· |
| (b) Detector resolution | 0.01 | 0.2 | 0.01 | 0.1 |
| (c) Low-energy tail | 0.03 | 0.1 | 0.03 | 0.1 |
| (d) Fitting robustness | 0.05 | 0.3 | 0.05 | 0.3 |

# Number of spectra - SIDDHARTA-2 2022 Run

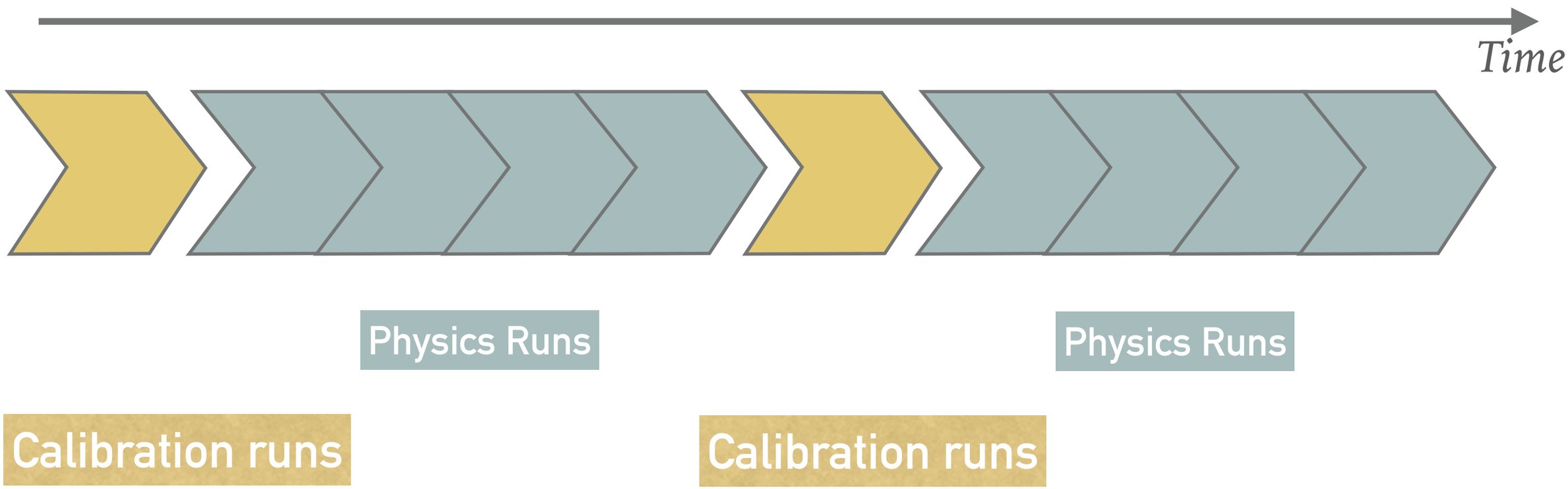
See S. Manti talk




Calibration of SDD depends on:

- Availability of calibration runs (depends on machine conditions/availability) (Ideally one wants the beam on 24/7)
- Dependence on temperature/pressure @ the detectors
  - Not precisely know (vacuum, cryo conditions, setup constraints)
- Dependence on beam background

# Typical calibration strategy




*Need to balance - trade off!*

*Want more calibration points*
*but also more physics data*

# *Enhance calibrations to the limit with differentiable programming*

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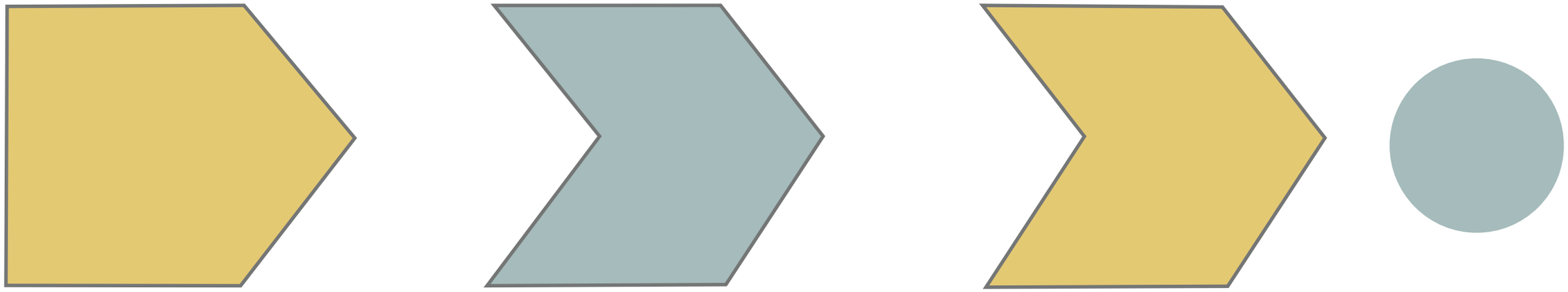


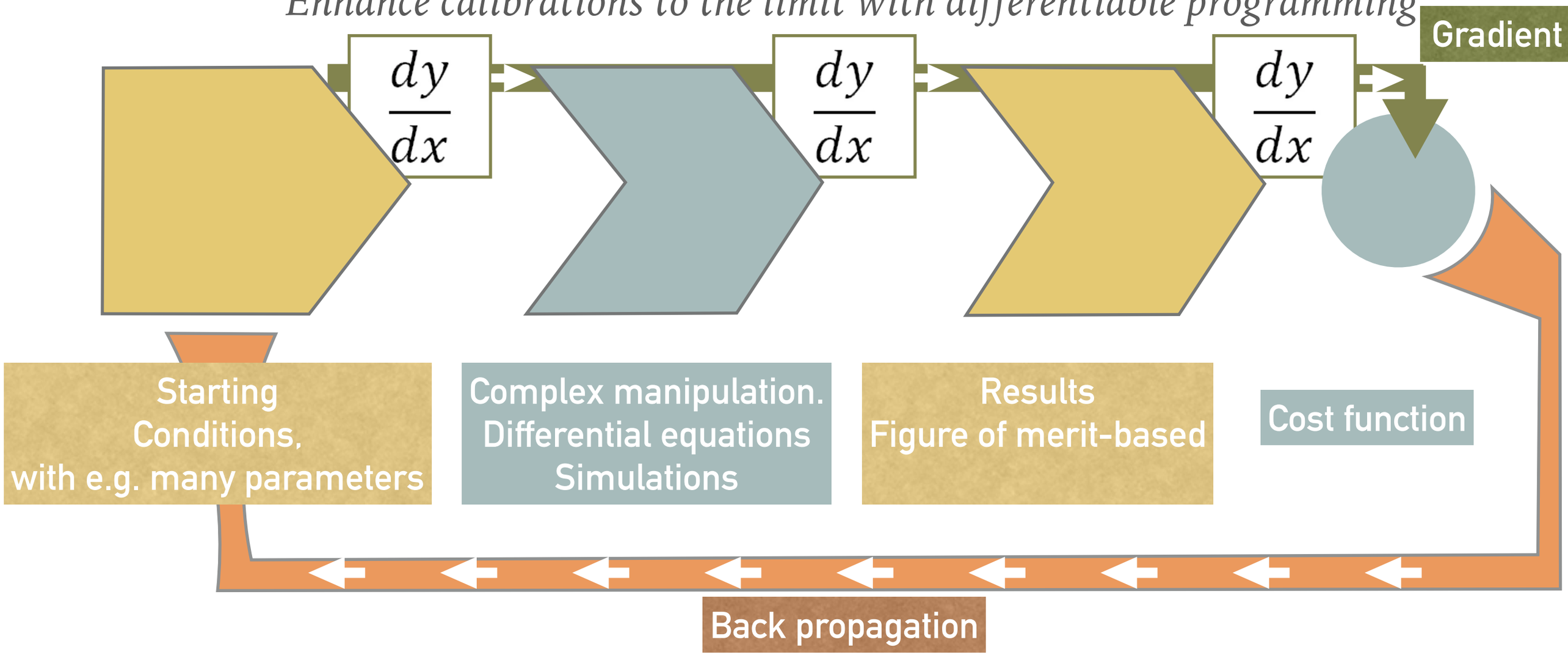
Starting Conditions, with e.g. many parameters

Complex manipulation. Differential equations Simulations

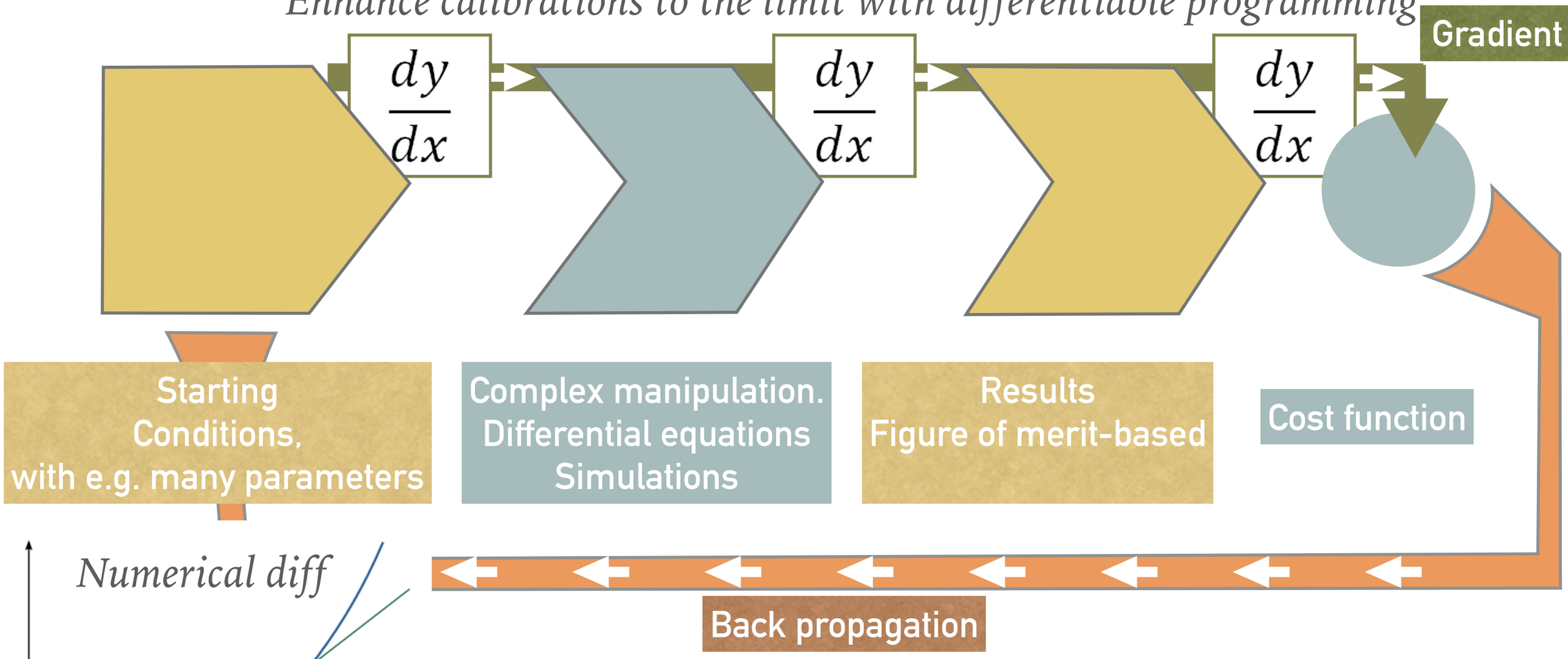
Results Figure of merit-based

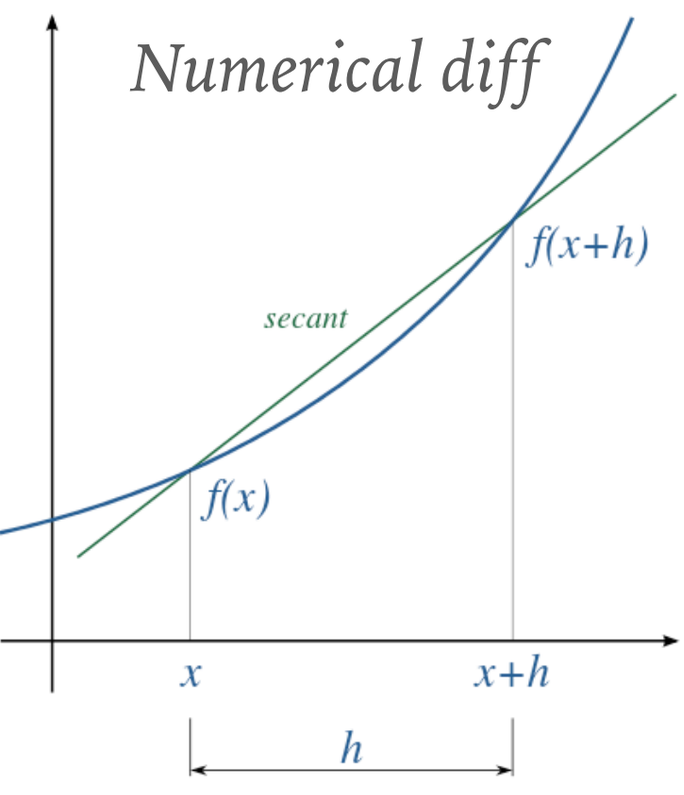
Cost function

*Enhance calibrations to the limit with differentiable programming*

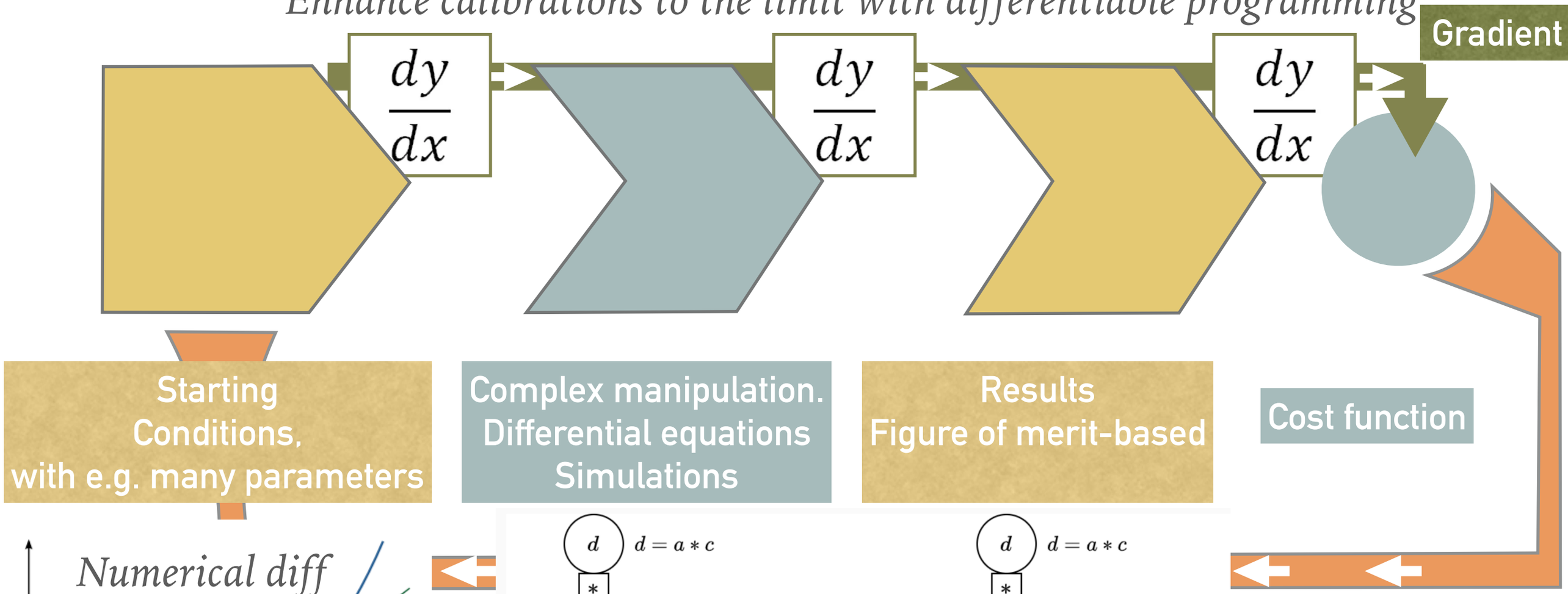


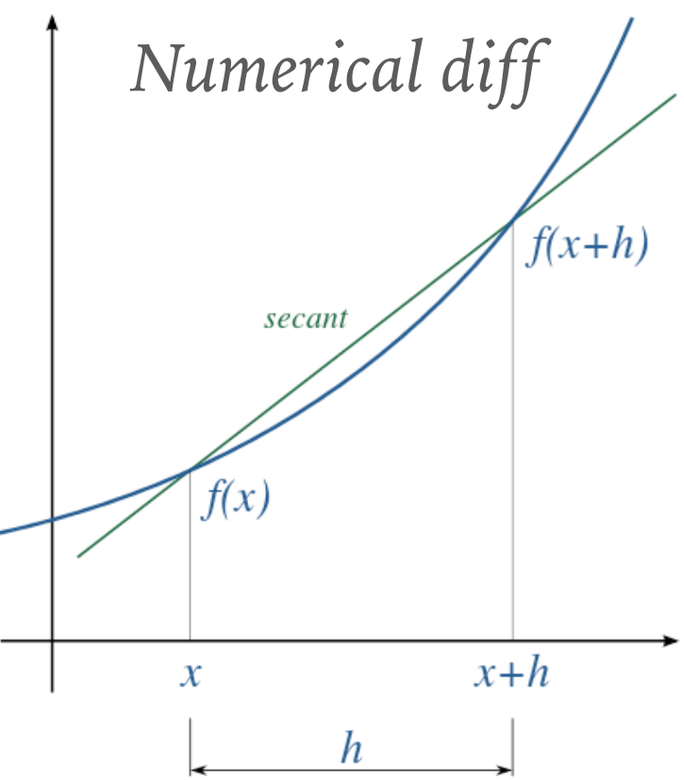
# Enhance calibrations to the limit with differentiable programming

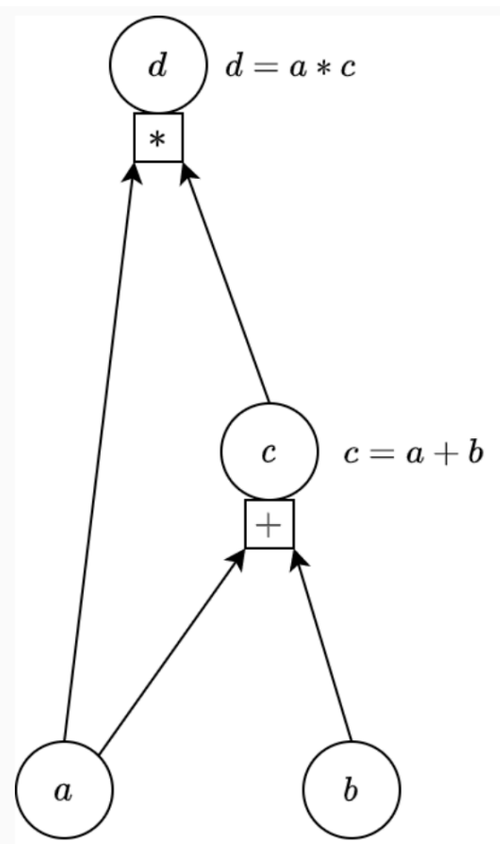


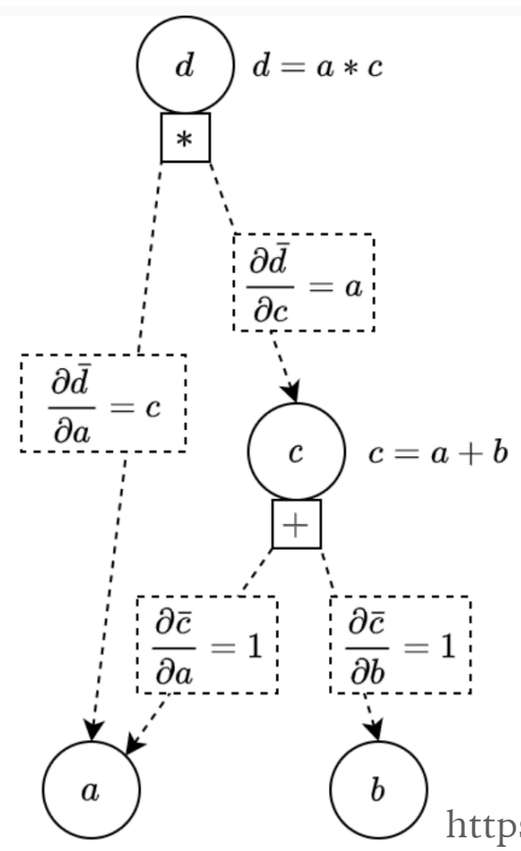



# Enhance calibrations to the limit with differentiable programming




$$\frac{\partial d}{\partial a} = \frac{\partial \bar{d}}{\partial a} + \frac{\partial \bar{d}}{\partial c} * \frac{\partial \bar{c}}{\partial a}$$

$$\frac{\partial d}{\partial a} = c + a * 1$$

$$\frac{\partial d}{\partial a} = a + b + a$$

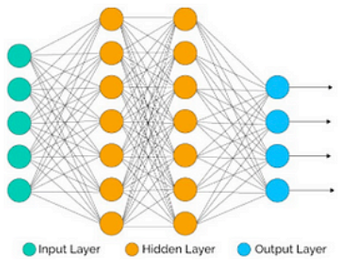
$$\frac{\partial d}{\partial a} = 2a + b$$

https://sidsite.com/posts/autodiff/

# Enhance calibrations to the limit with differentiable programming

Target and environment variables → Neural Network → Control Parameters → ODE Solver → Loss

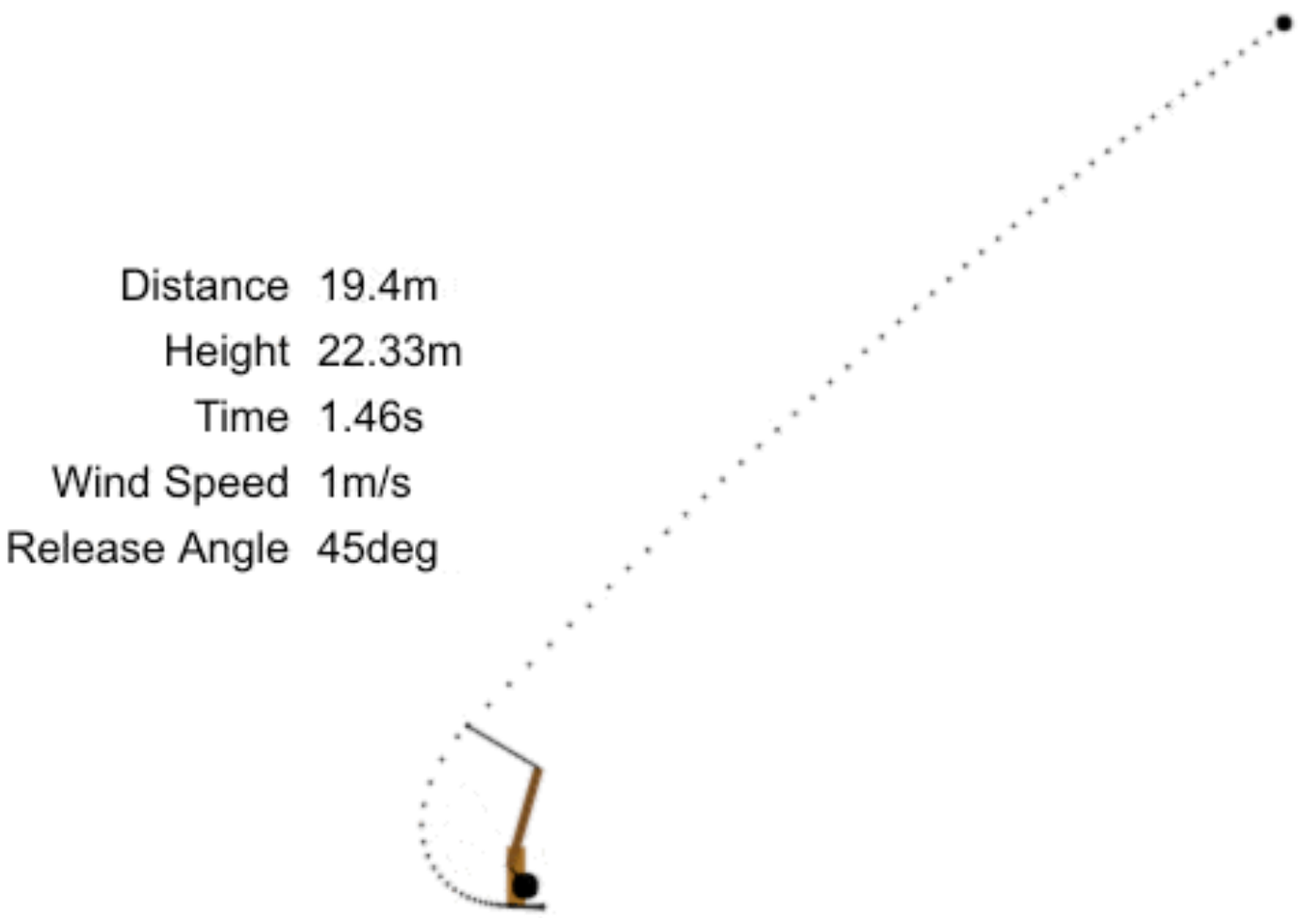
*wind = -10m/s*
*target = 50m*




*angle = 25°*
*weight = 200kg*

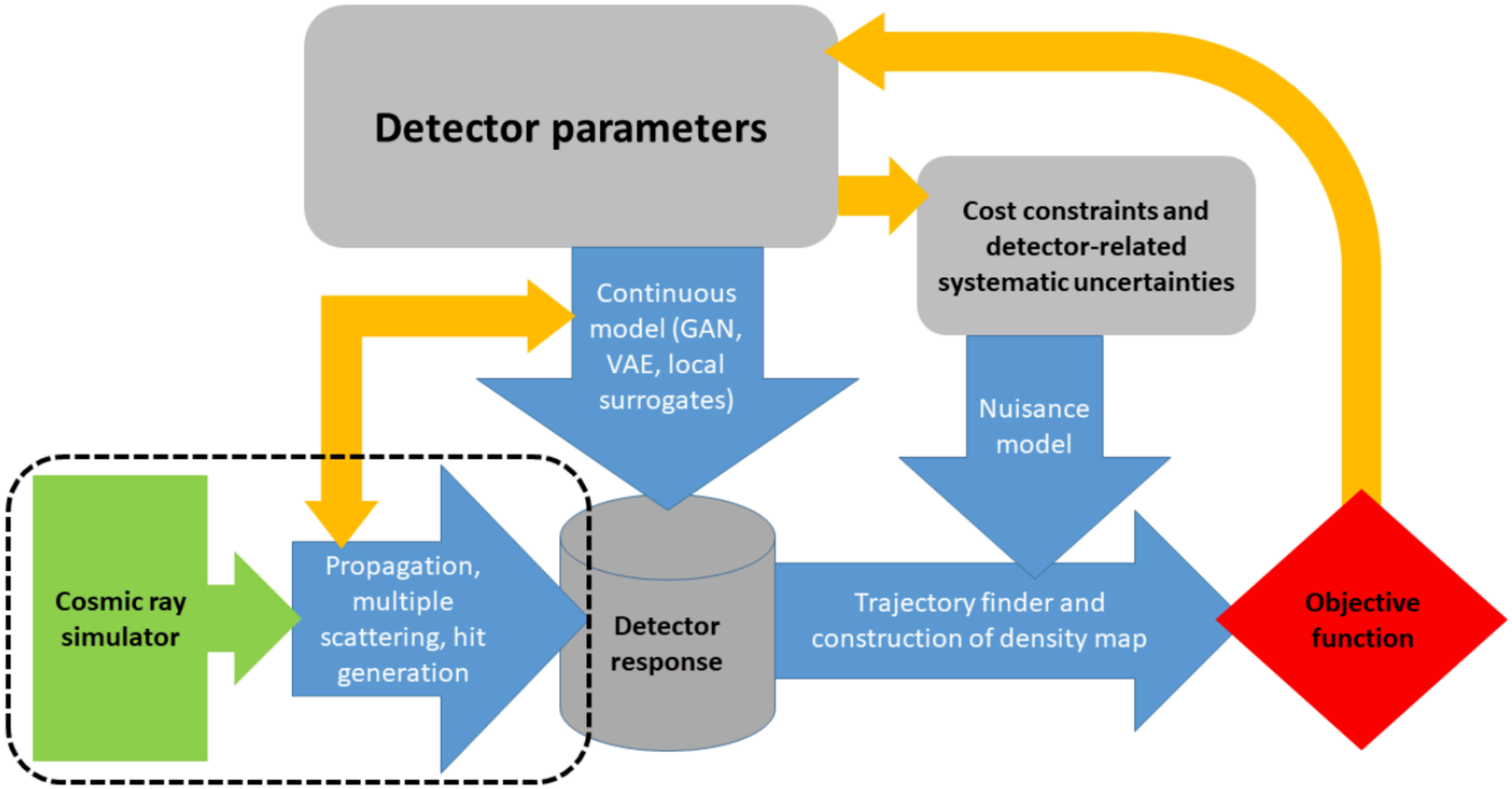
*(target_distance − actual_distance)²*

Backpropagation




https://github.com/JuliaComputing/ODSC2019

# Enhance calibrations to the limit with differentiable programming

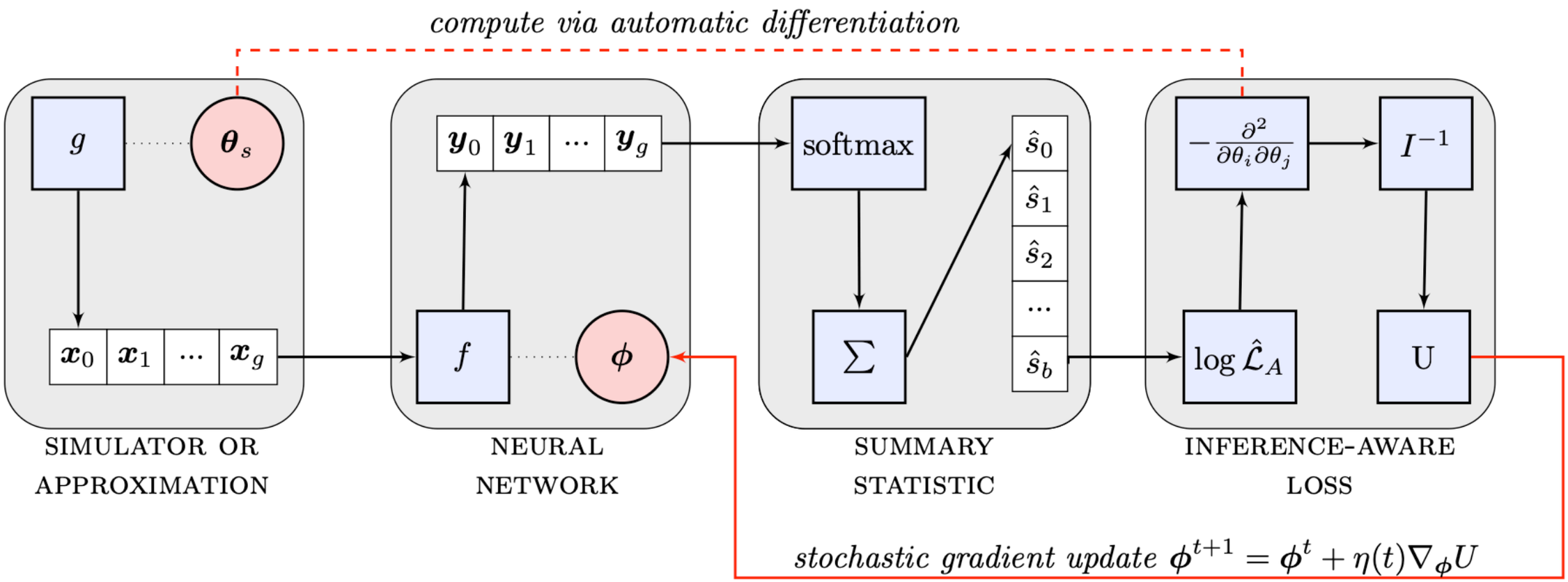



- Optimization of detector design and operation

MODE
Machine-learning Optimized Design of Experiments

https://inspirehep.net/files/8f6784eac6a7f06c184cfc50757de656

# Enhance calibrations to the limit with differentiable programming

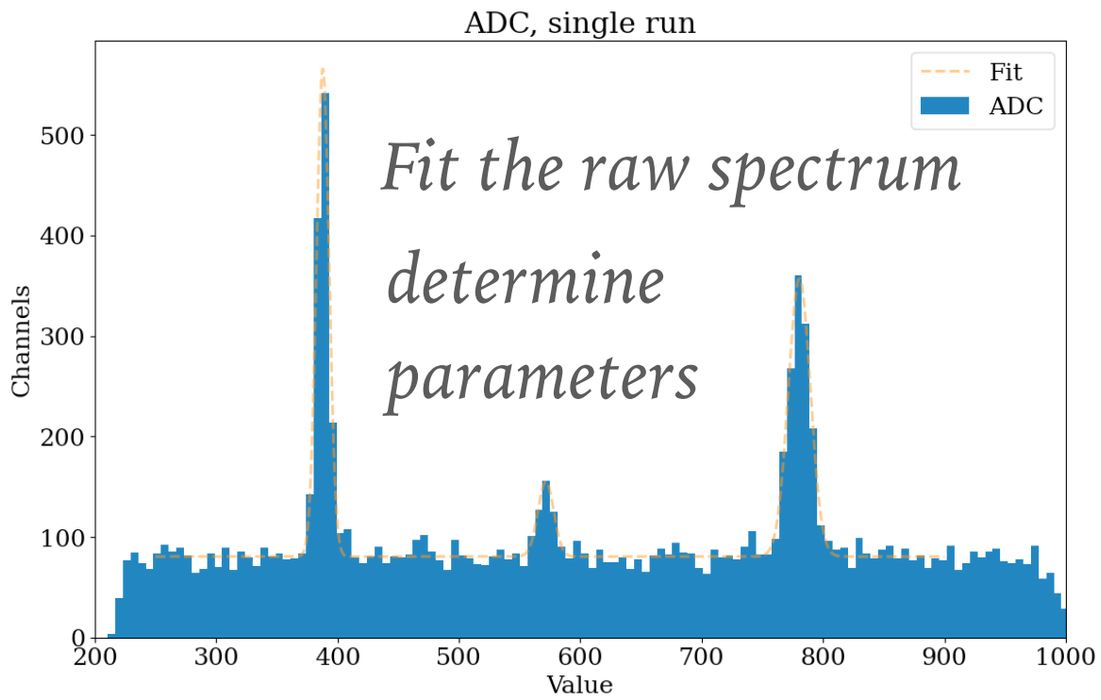


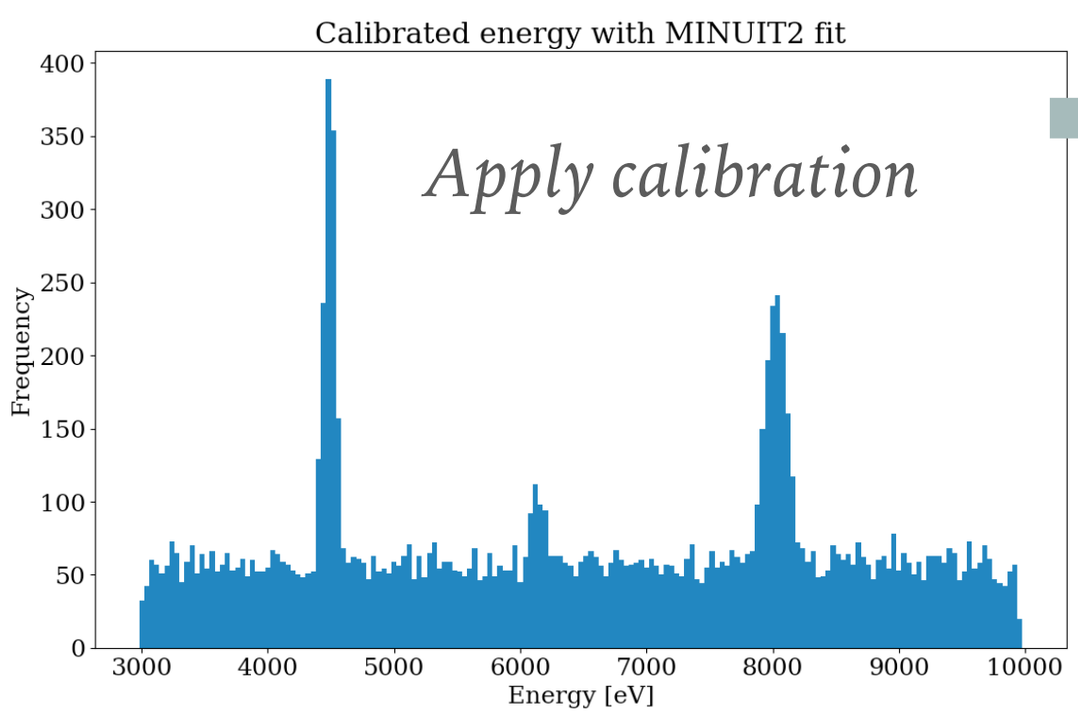

Sketch of the INFERNO algorithm. Batches from a simulator are passed through a neural network and a differentiable summary statistic is constructed that allows to calculate the variance of the POI. The parameters of the network are then updated by stochastic gradient descent.

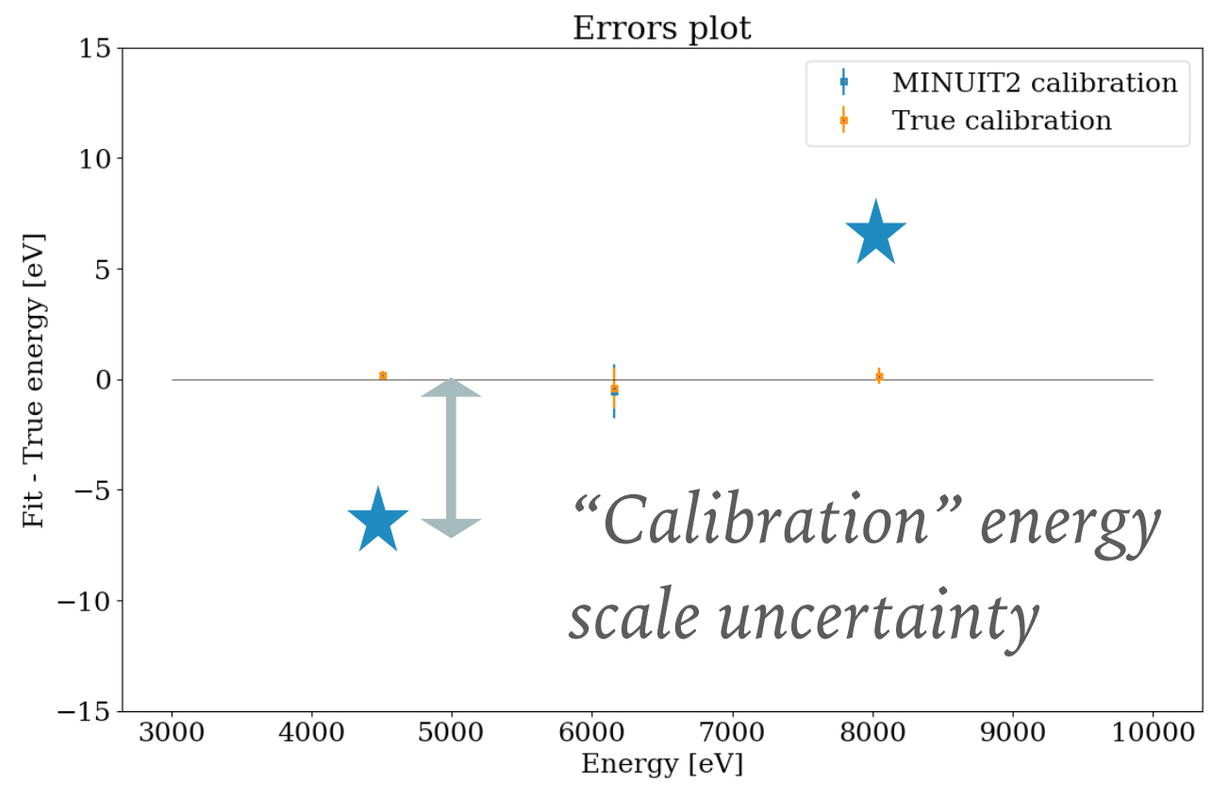
https://cds.cern.ch/record/2807001/plots

# A test optimisation setup

## The "Standard Approach" to spectroscopic calibration



# A test optimisation setup

The differentiable programming approach

## Loss function for the gradient: loss

**Take new calibration constants**

$$\mathbf{E} = \mathscr{C}(\mathbf{ADC} \,|\, \mathbf{P})$$

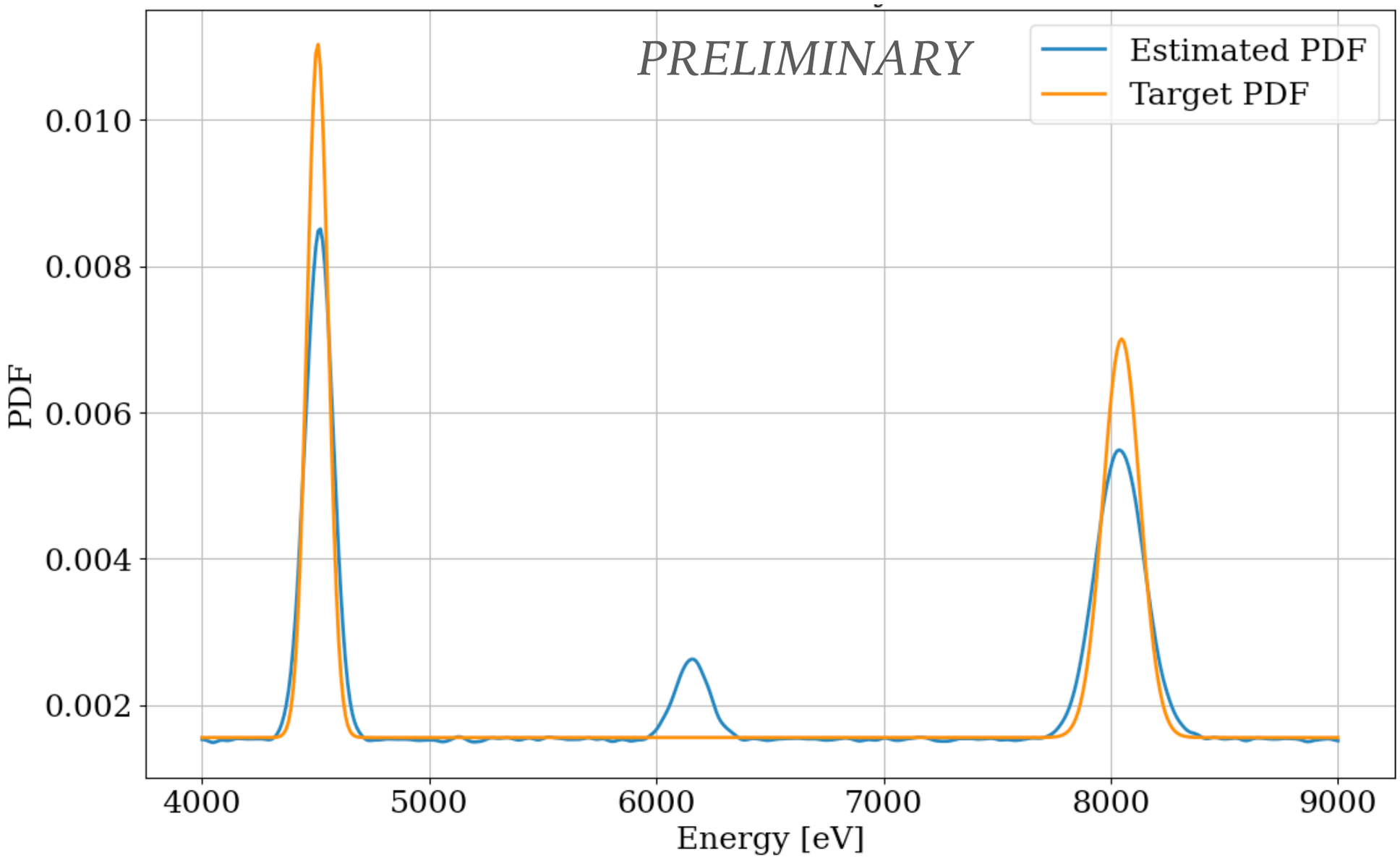
**Derive calibrated dataset**

$$\mathscr{L}(\mathbf{E})$$

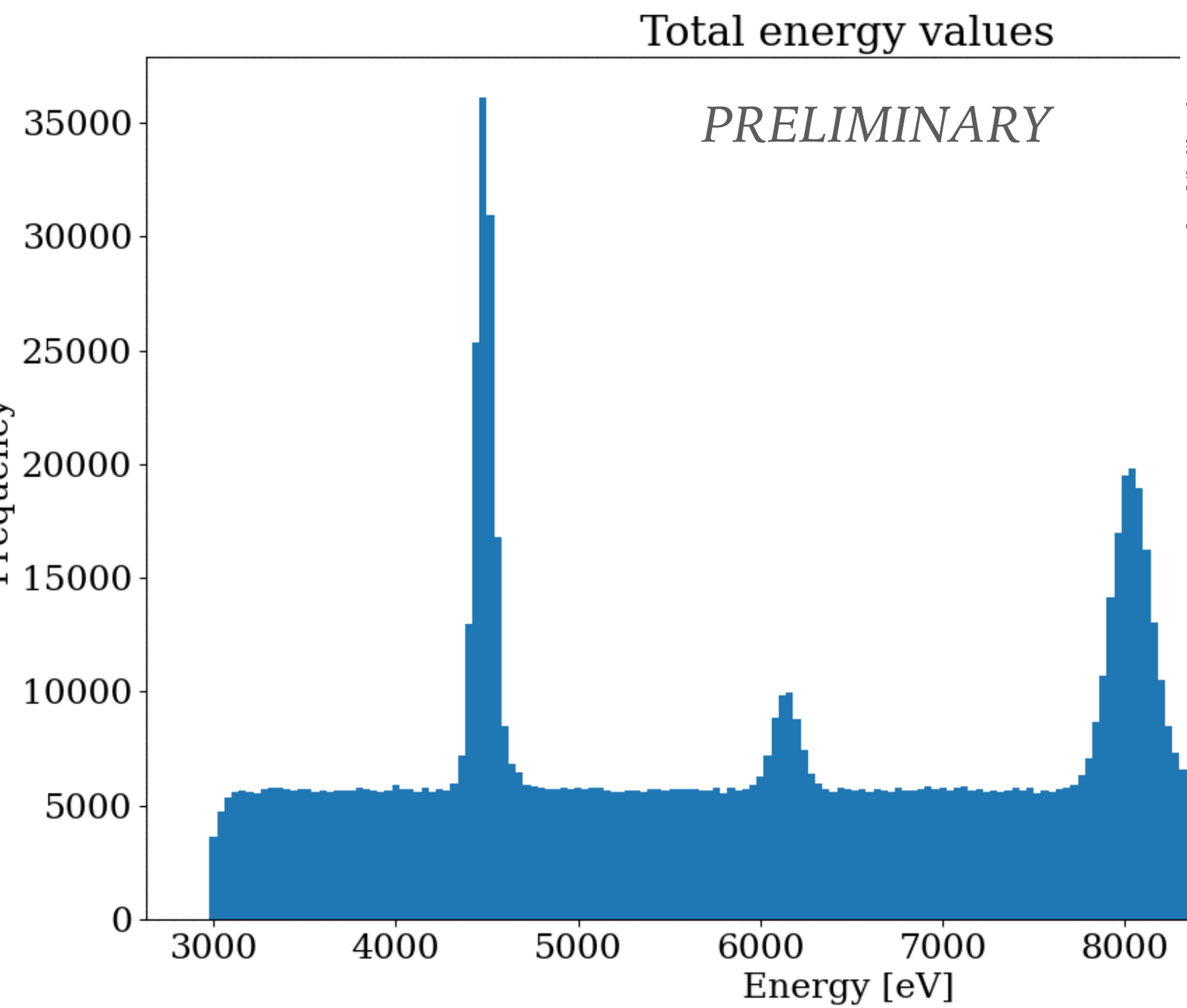
**Compute the loss**

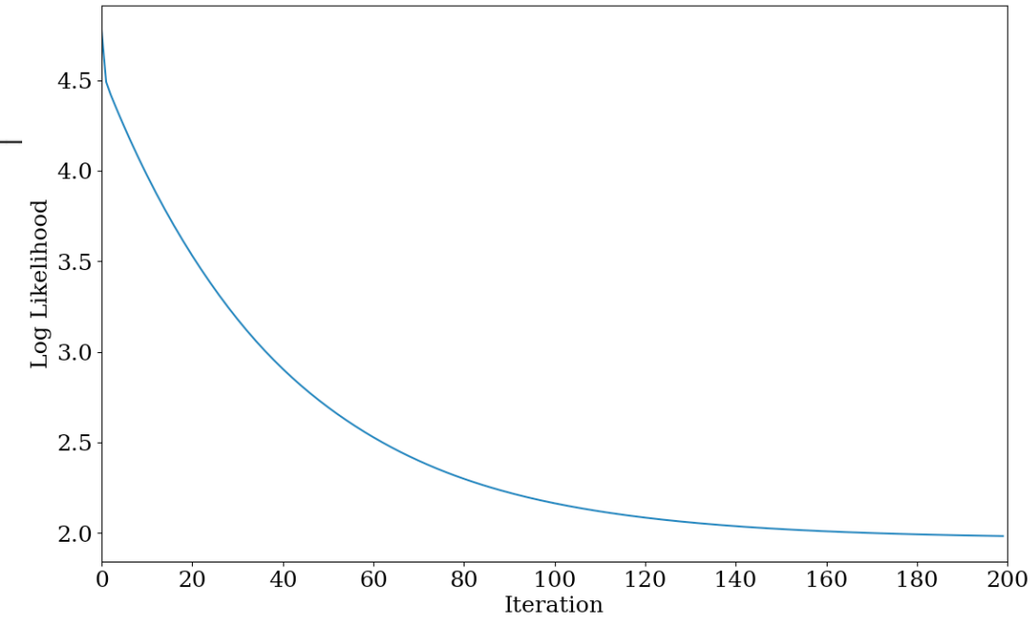
$$\mathbf{P} = \begin{bmatrix} p_{0,1} & p_{1,1} & p_{2,1} \\ \vdots & \vdots & \vdots \\ p_{0,i} & p_{1,i} & p_{2,i} \\ \vdots & \vdots & \vdots \\ p_{0,N} & p_{1,N} & p_{2,N} \end{bmatrix}$$

**Update P to minimize the loss**

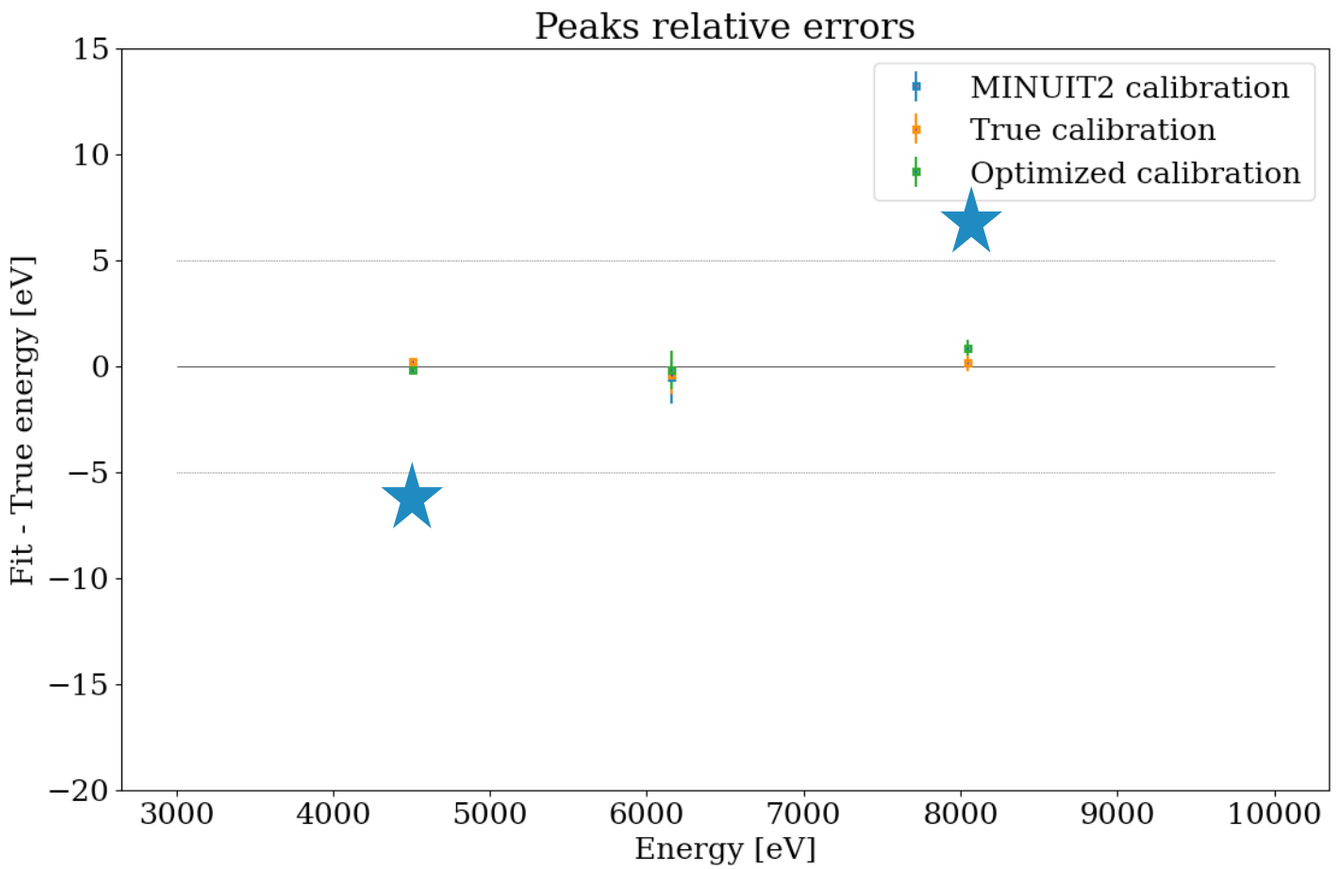



*Distance to target PDF estimated via KDE approximation*


Total energy values
PRELIMINARY
Frequency
35000
30000
25000
20000
15000
10000
5000
0
3000
4000
5000
6000
7000
8000
9000
10000
Energy [eV]

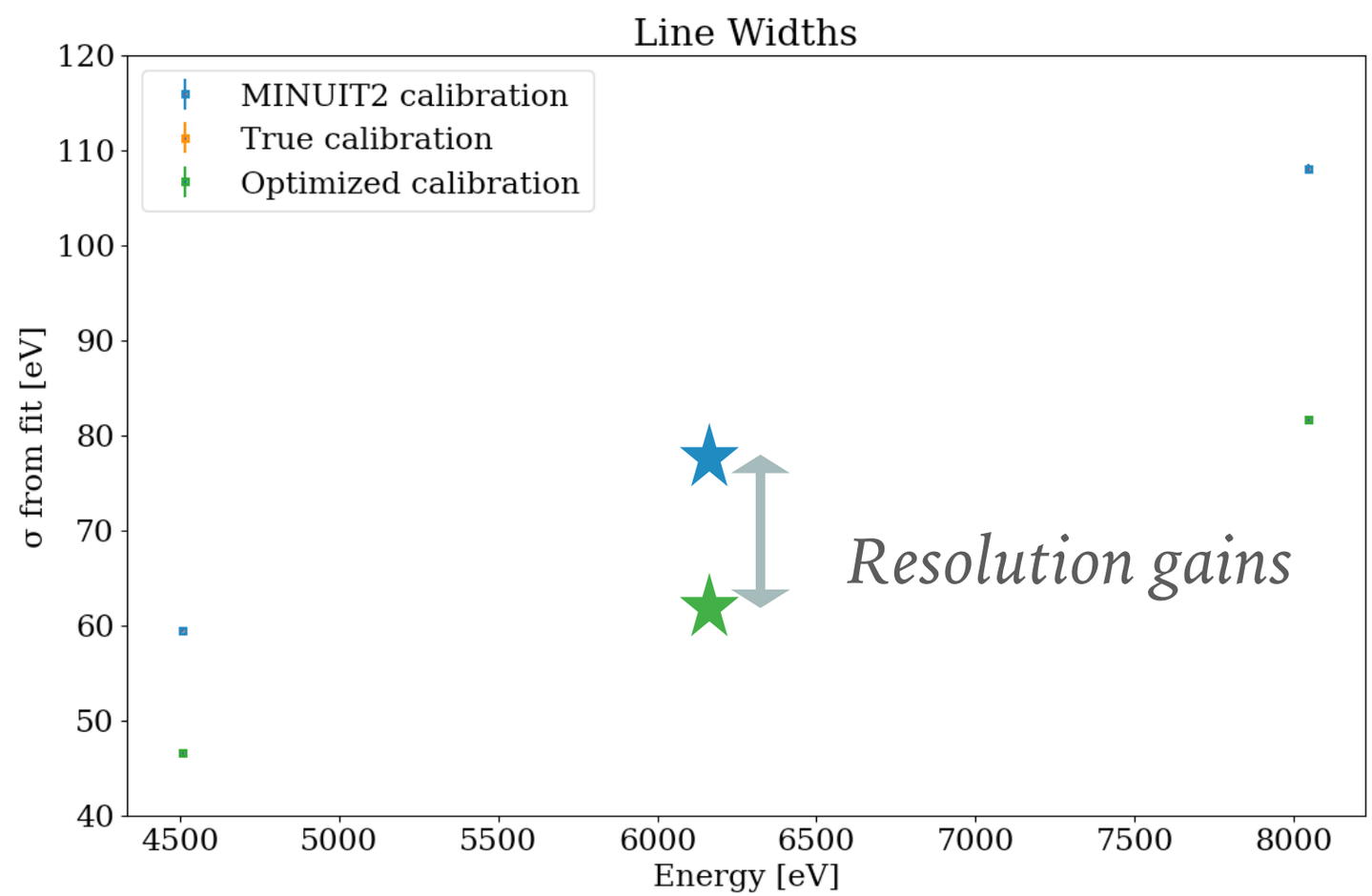

Log Likelihood
4.5
4.0
3.5
3.0
2.5
2.0
0
20
40
60
80
100
120
140
160
180
200
Iteration

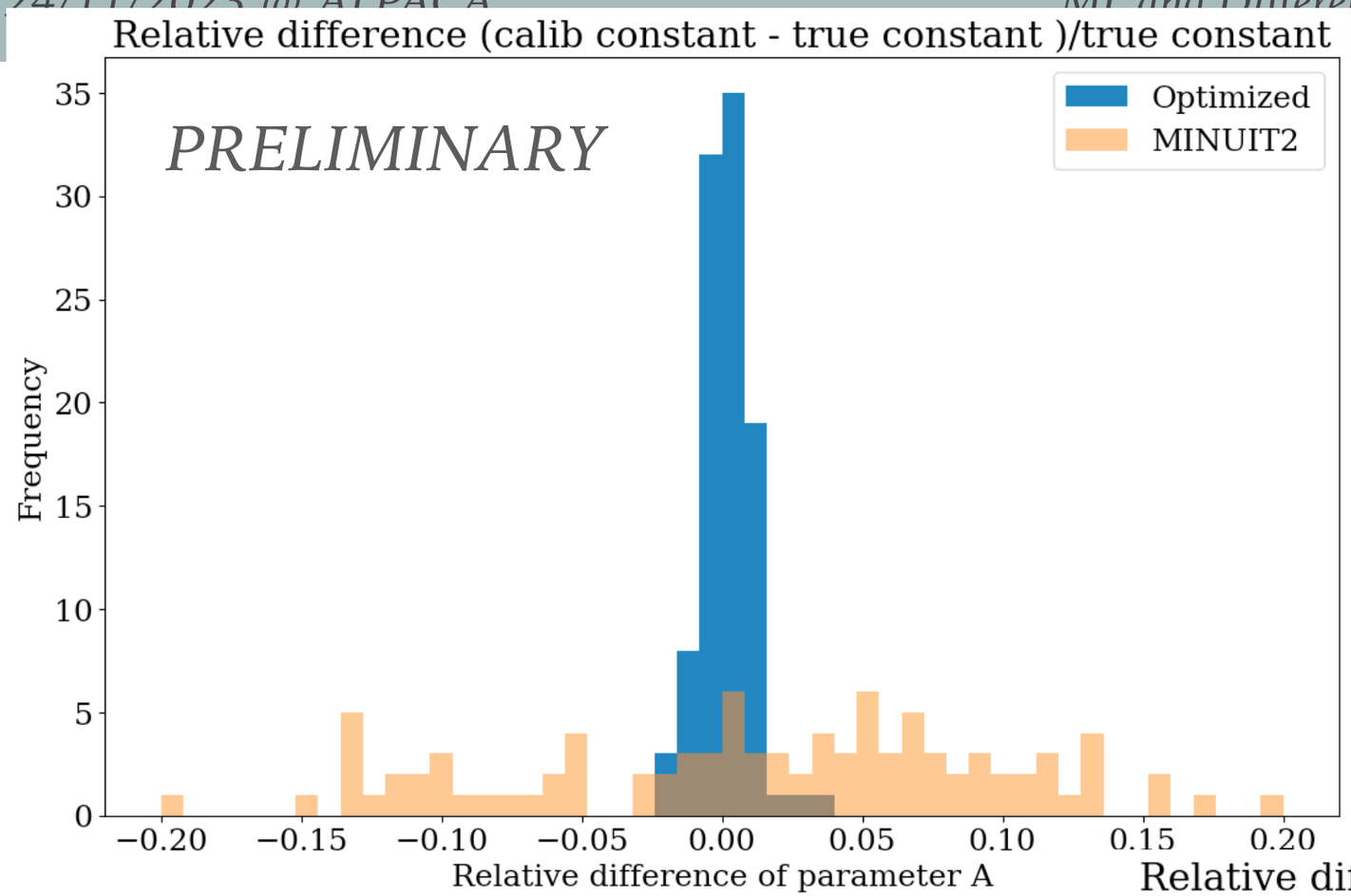
PRELIMINARY

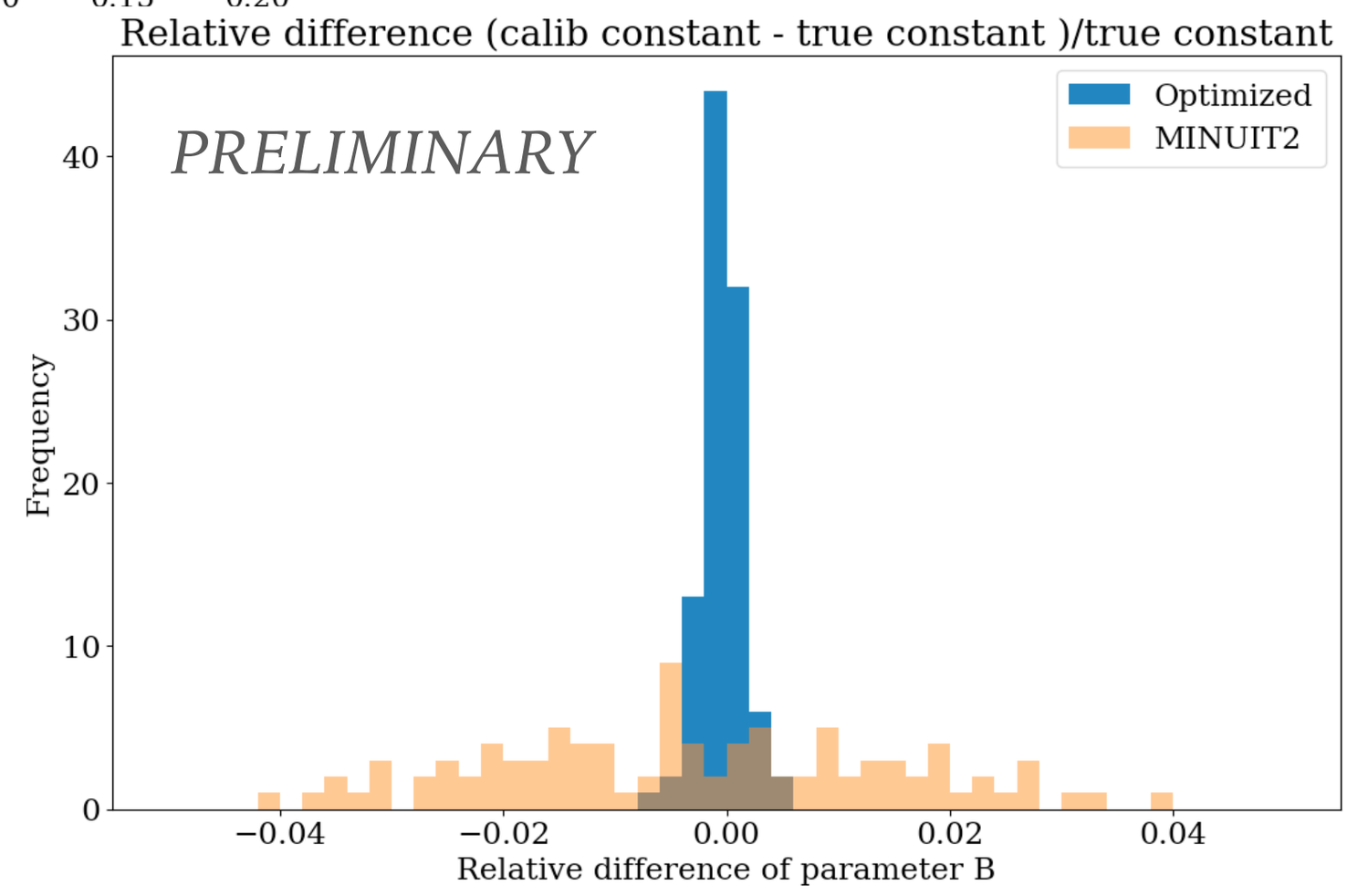



*Minimize the uncertainty to the statistical level*

*Nice gains in spectroscopic peaks resolution*

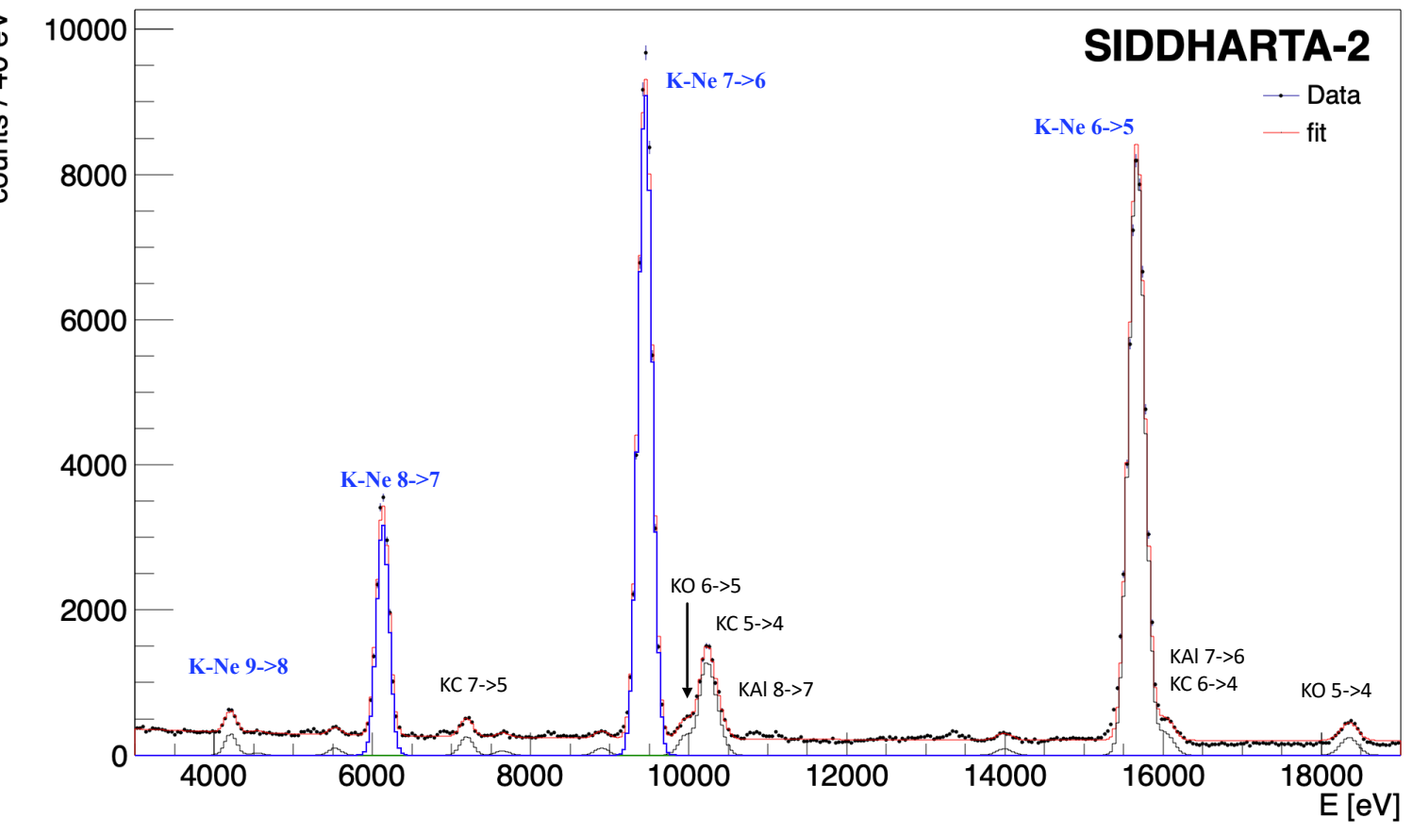


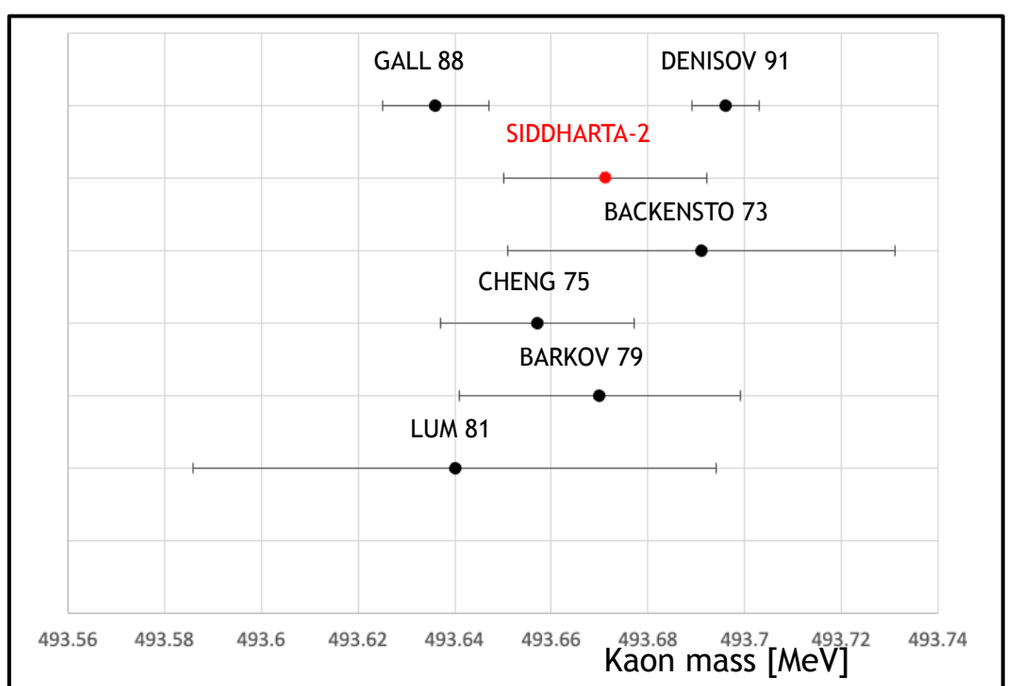

Relative difference (calib constant - true constant )/true constant
PRELIMINARY
Optimized
MINUIT2
Frequency
0
5
10
15
20
25
30
35
−0.20
−0.15
−0.10
−0.05
0.00
0.05
0.10
0.15
0.20
Relative difference of parameter A

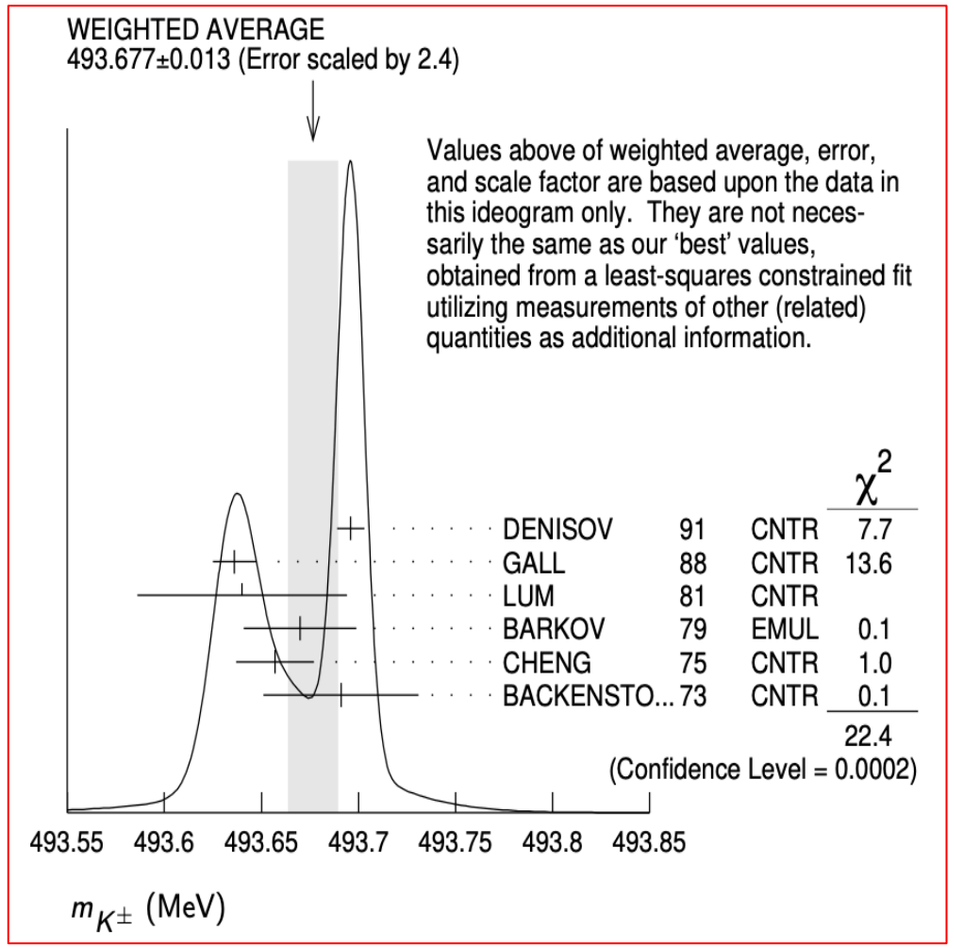

Relative difference (calib constant - true constant )/true constant
PRELIMINARY
Optimized
MINUIT2
Frequency
0
10
20
30
40
−0.04
−0.02
0.00
0.02
0.04
Relative difference of parameter B

# Outlook: kaon mass measurement @ SIDDHARTA-2

| Line | Energy [eV] |
|---|---|
| **K-Ne 98** | 4206.35 3.75 (stat) |
| **K-Ne 8** | 6130.86 0.71 (stat) 2 (sys.) |
| **K-Ne 7** | 9450.08 0.41 (stat) 2 (sys.) |
| **K-Ne 6** | 15673.30 0.52 (stat) 5 (sys.) |



# Conclusions

- Calibration is a critical source of uncertainty in spectroscopy x-ray experiment
- Differentiable prog. approach has the potential to minimize
  - Can enhance existing data
  - Can calibrate "intermediately" or at each step
- In principle applicable to spectroscopic experiments
- Plan to test the method on real data for kaon mass meas

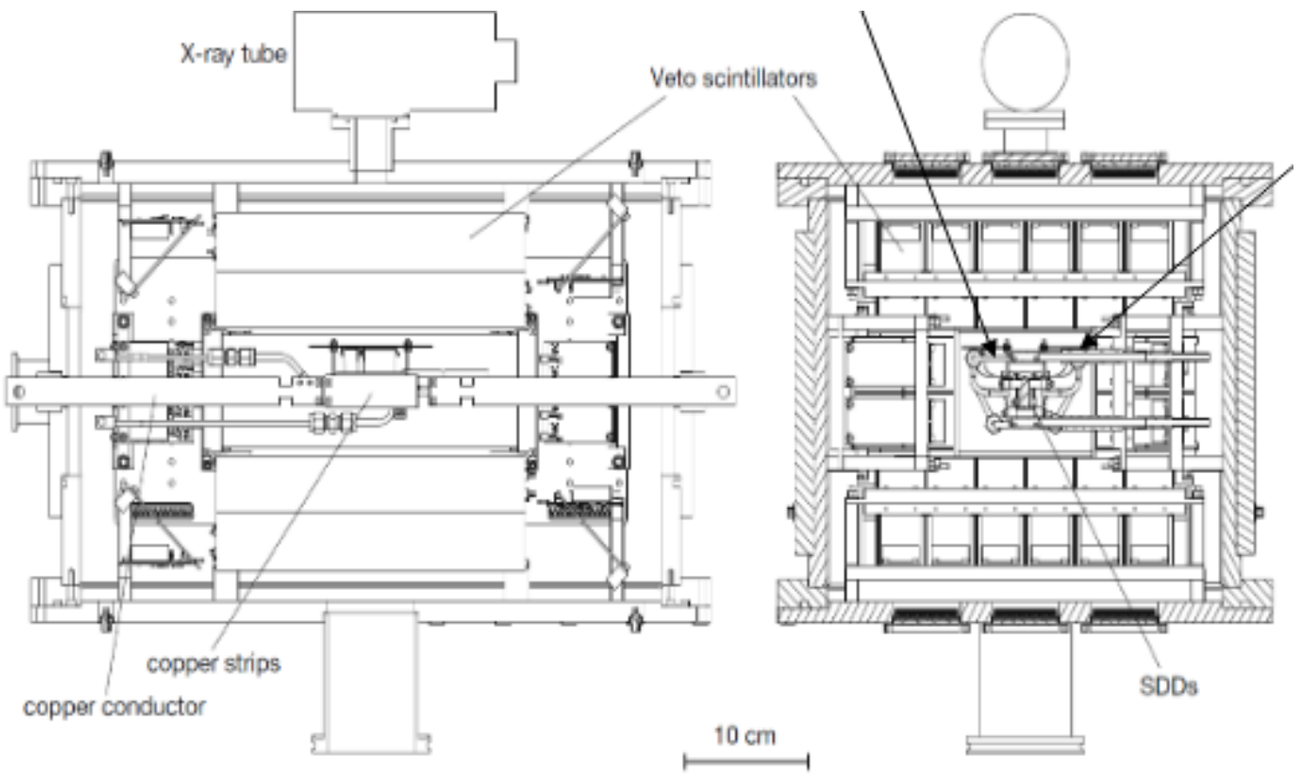
- Method based on: https://iopscience.iop.org/article/10.1088/1361-6501/ad080a/meta

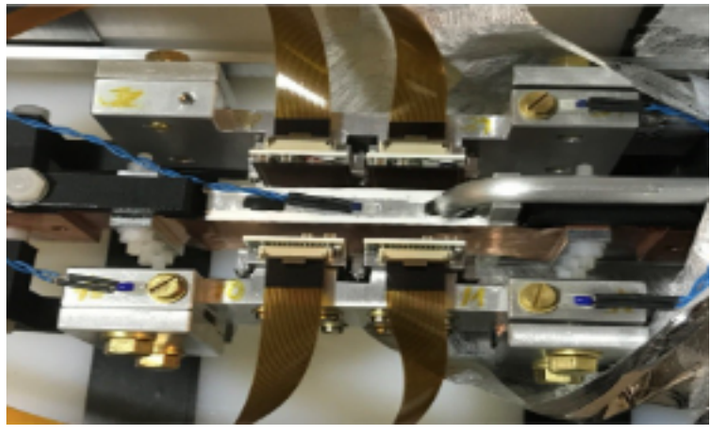
*Thank you for your attention!*

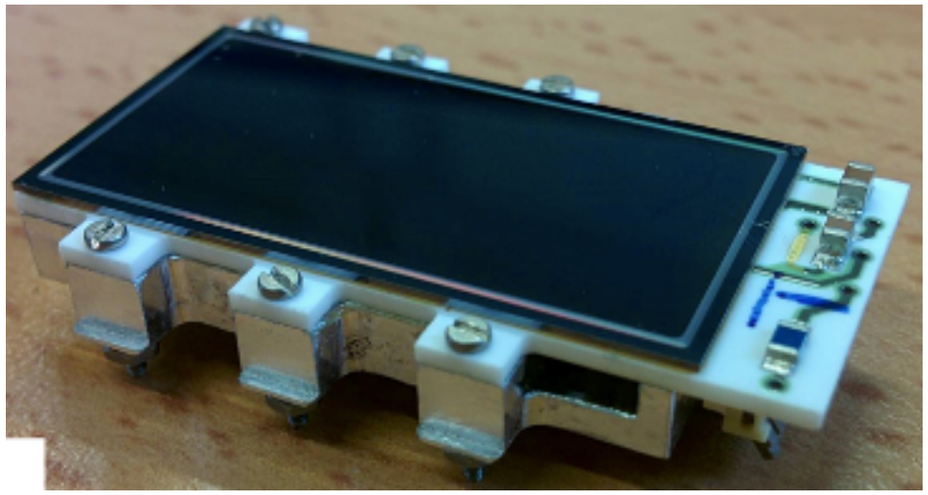
*Questions?*

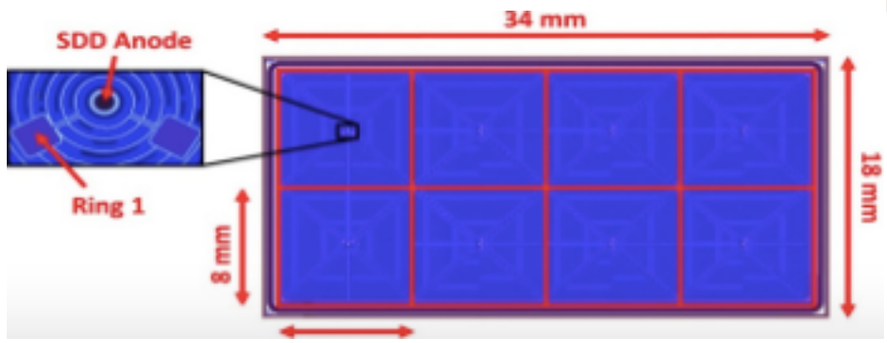
# The VIP-2 Experiment

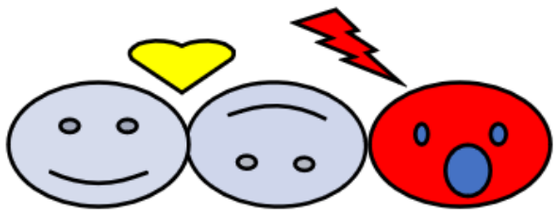
*Silicon Drift Detectors (**SDDs**) higher resolution (190 eV FWHM at 8.0 →keV), faster (triggerable) detectors. 4 arrays of 2 x 4 SDDs 8mm x 8mm each, liquid argon closed circuit cooling 170 °C*

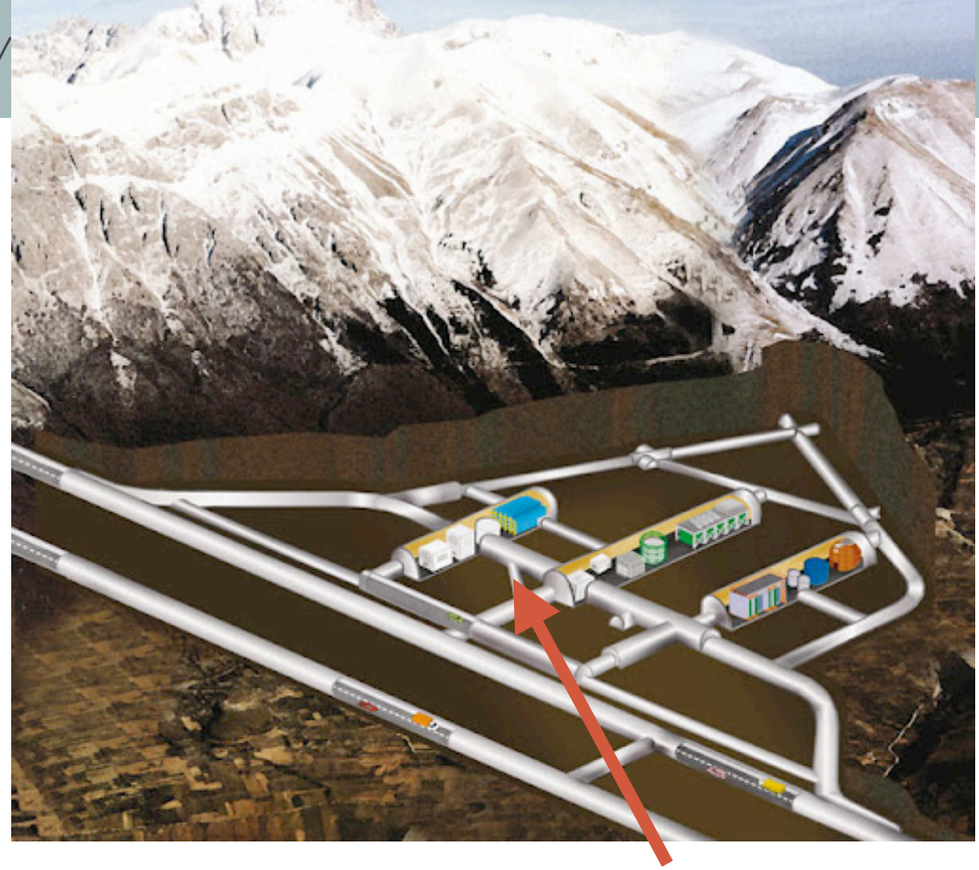




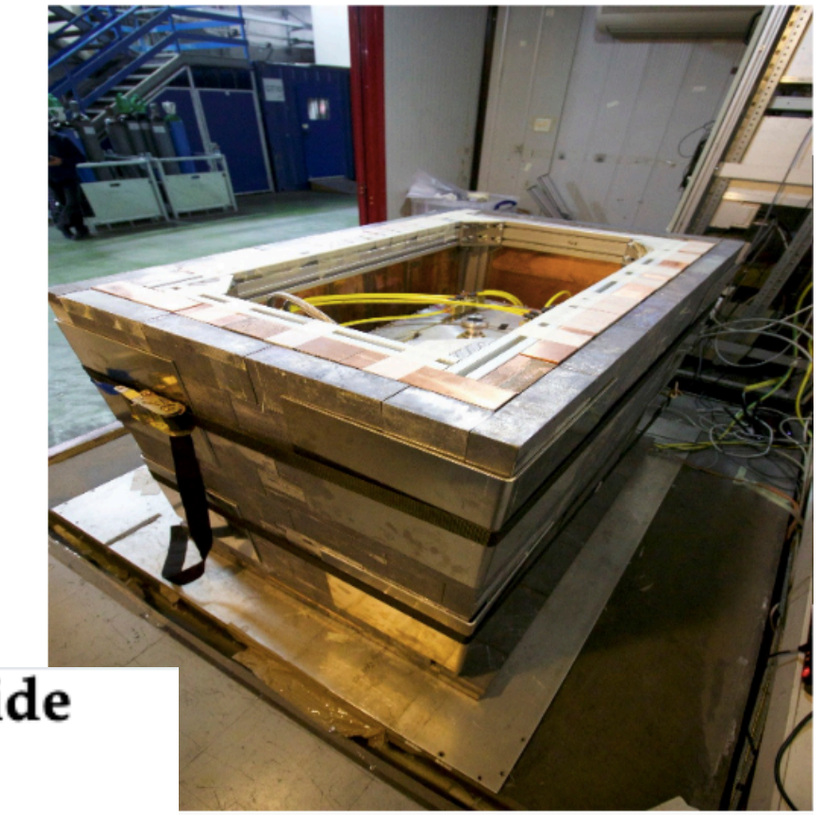


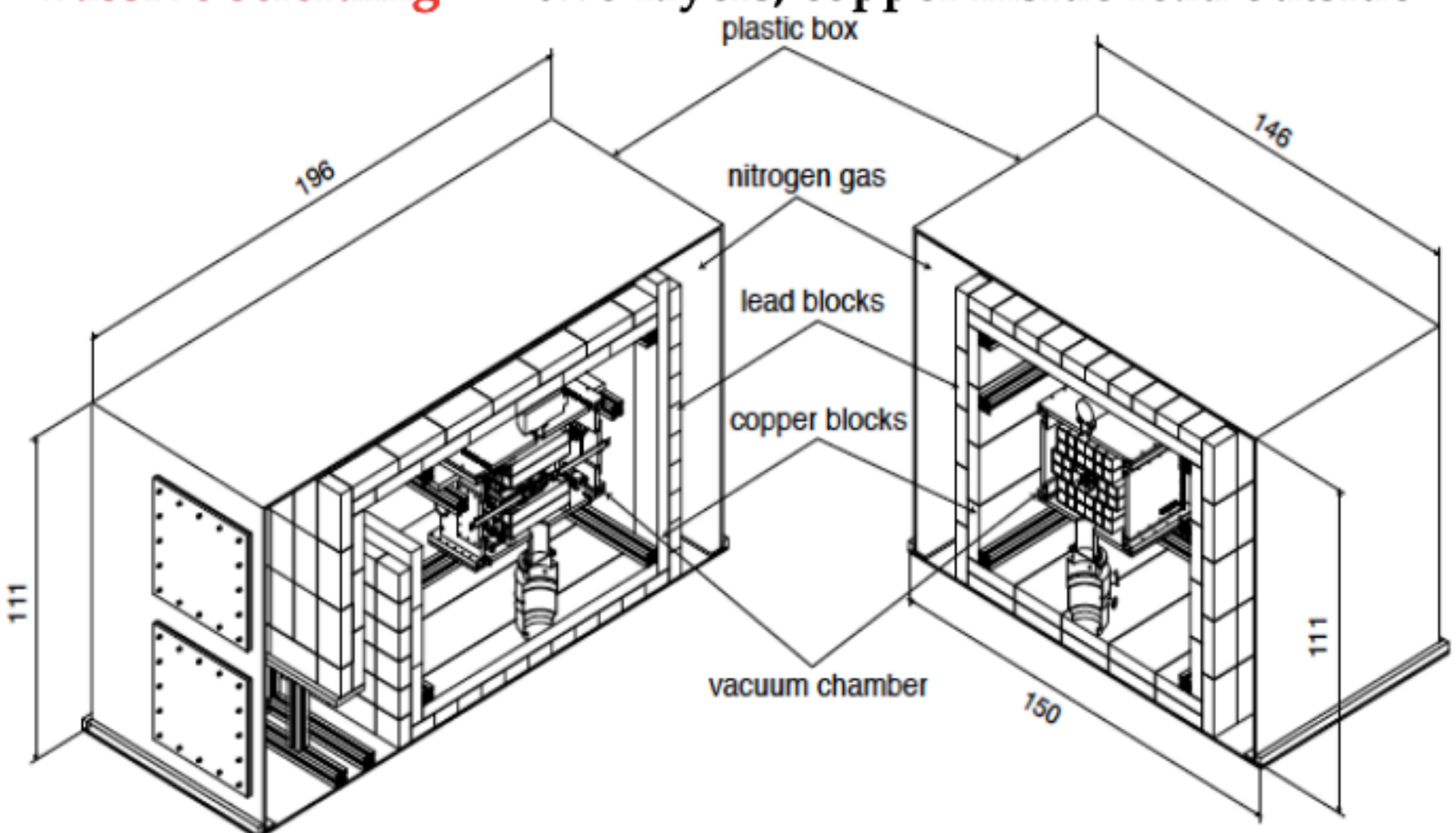


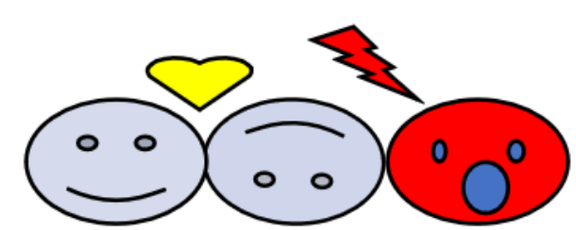
*1400 m rock coverage*

**Upgrade concluded in April 2019:**



**Passive scielding → two layers, copper inside lead outside**

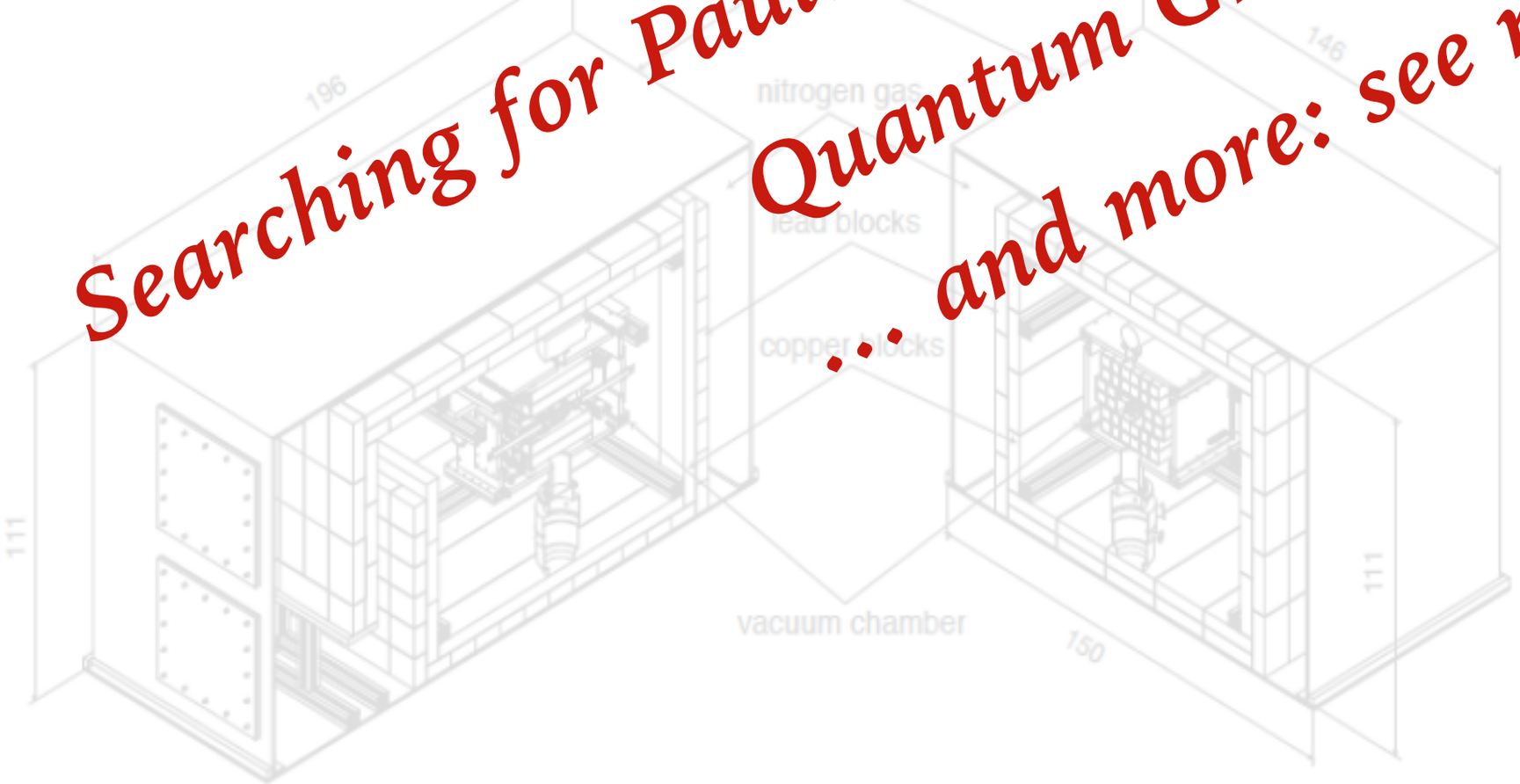


Upgrade concluded in April 2019:

1400 m rock
average

Passive scielding → two layers, copper inside lead outside

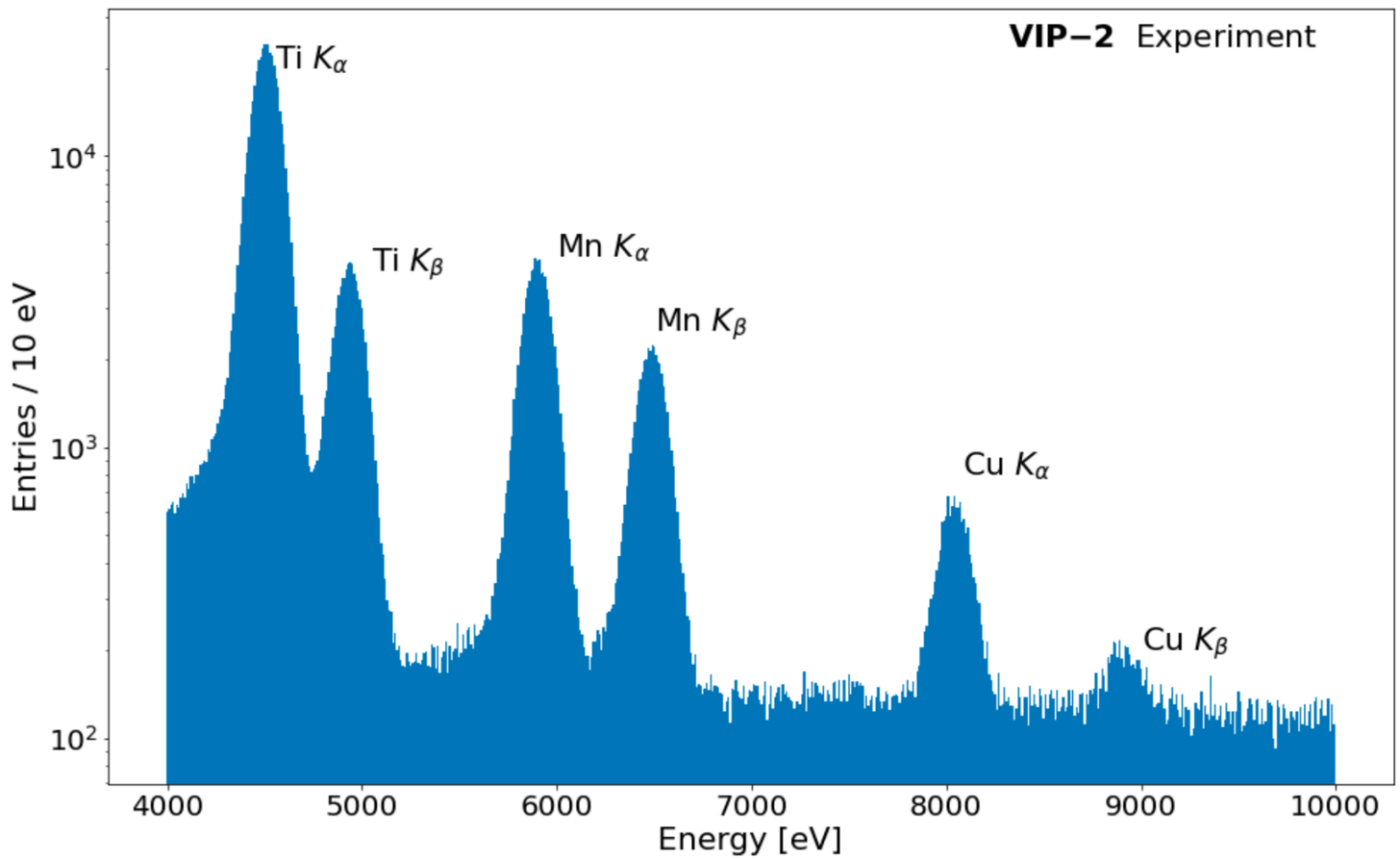



*Ideal place for precision X-ray spectroscopy*

*Searching for Pauli Exclusion Principle Violations*

*Quantum Gravity*

*... and more: see next talks!*




*Calibrated spectrum of 4 SDD arrays.*

*Not easy to calibrate because:*

- *Copper line at orders of magnitude smaller than Ti and Mn*
- *Tiny distortions of FEE*

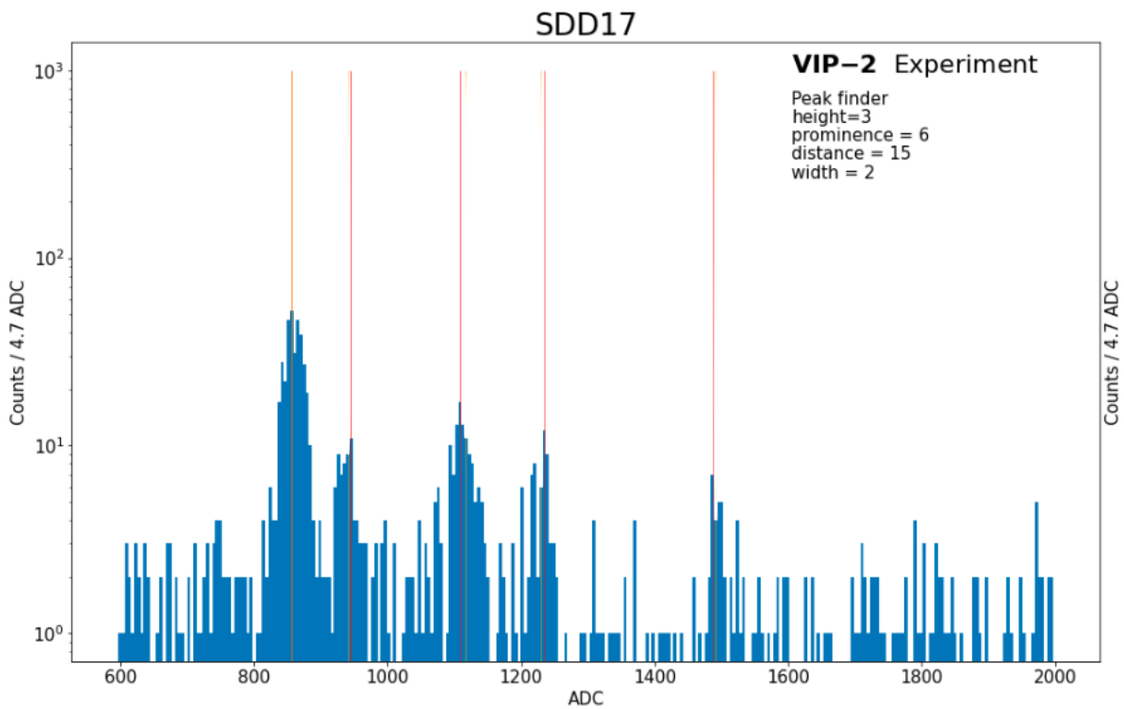
*Calibration can be done in big or small batches*

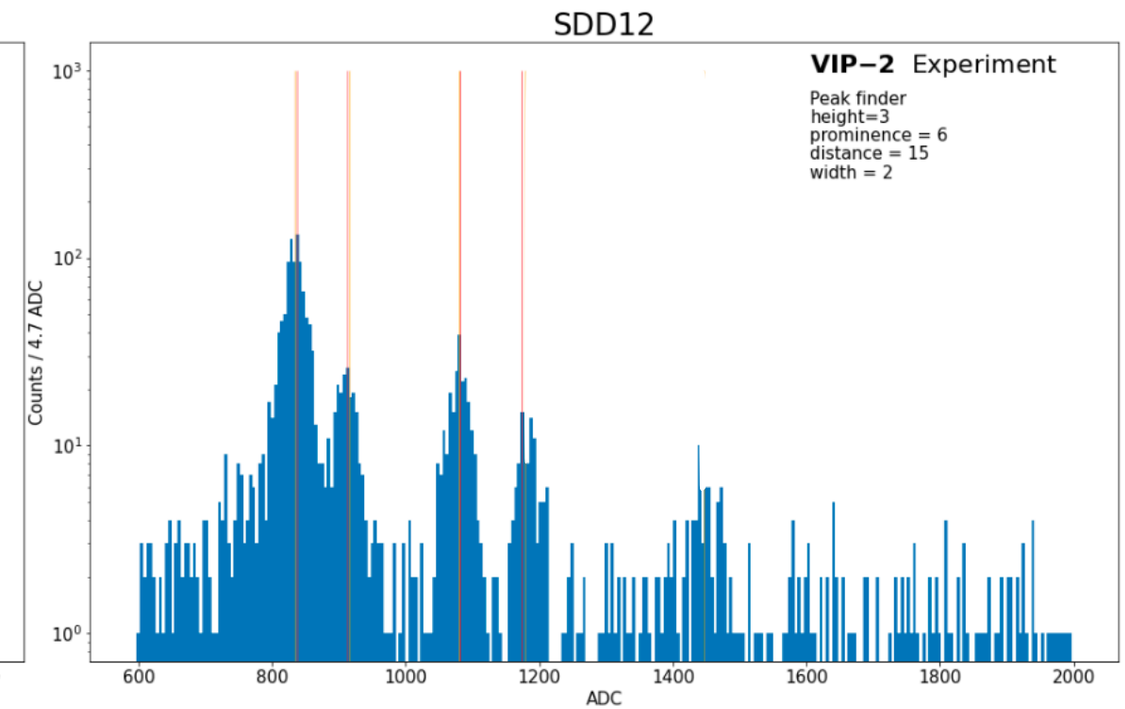
*Big batches*

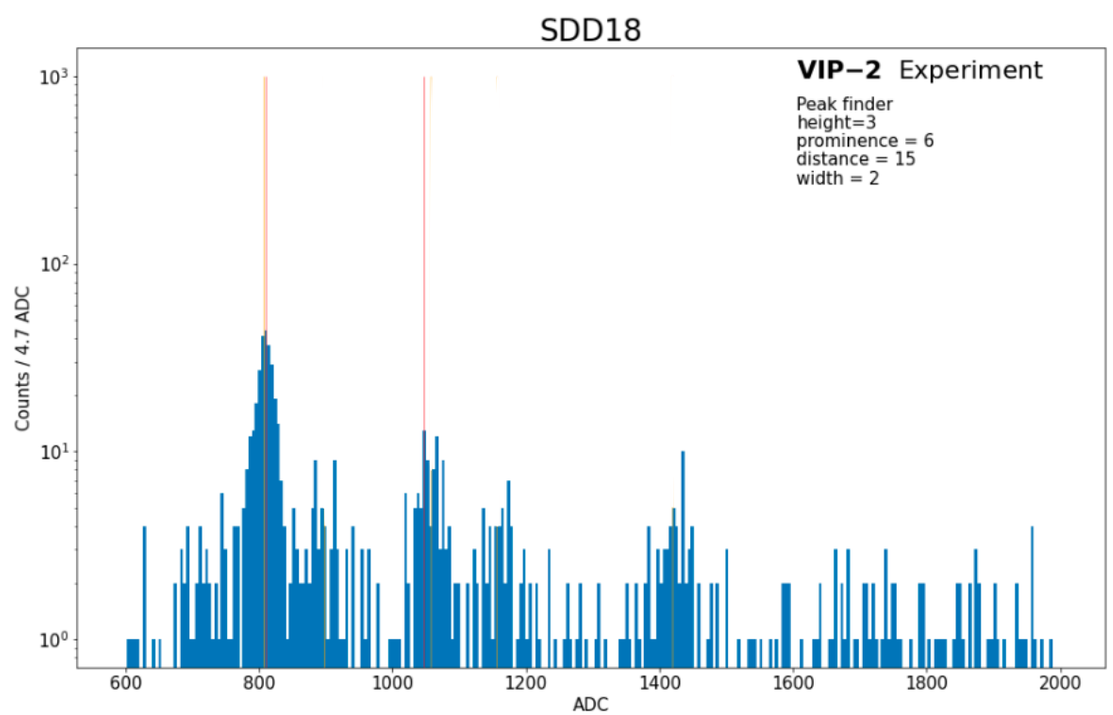
*Can determine better the Copper position but cannot capture fluctuations*

*Small batches*

*Can capture fluctuations but cannot determine the Copper position well*

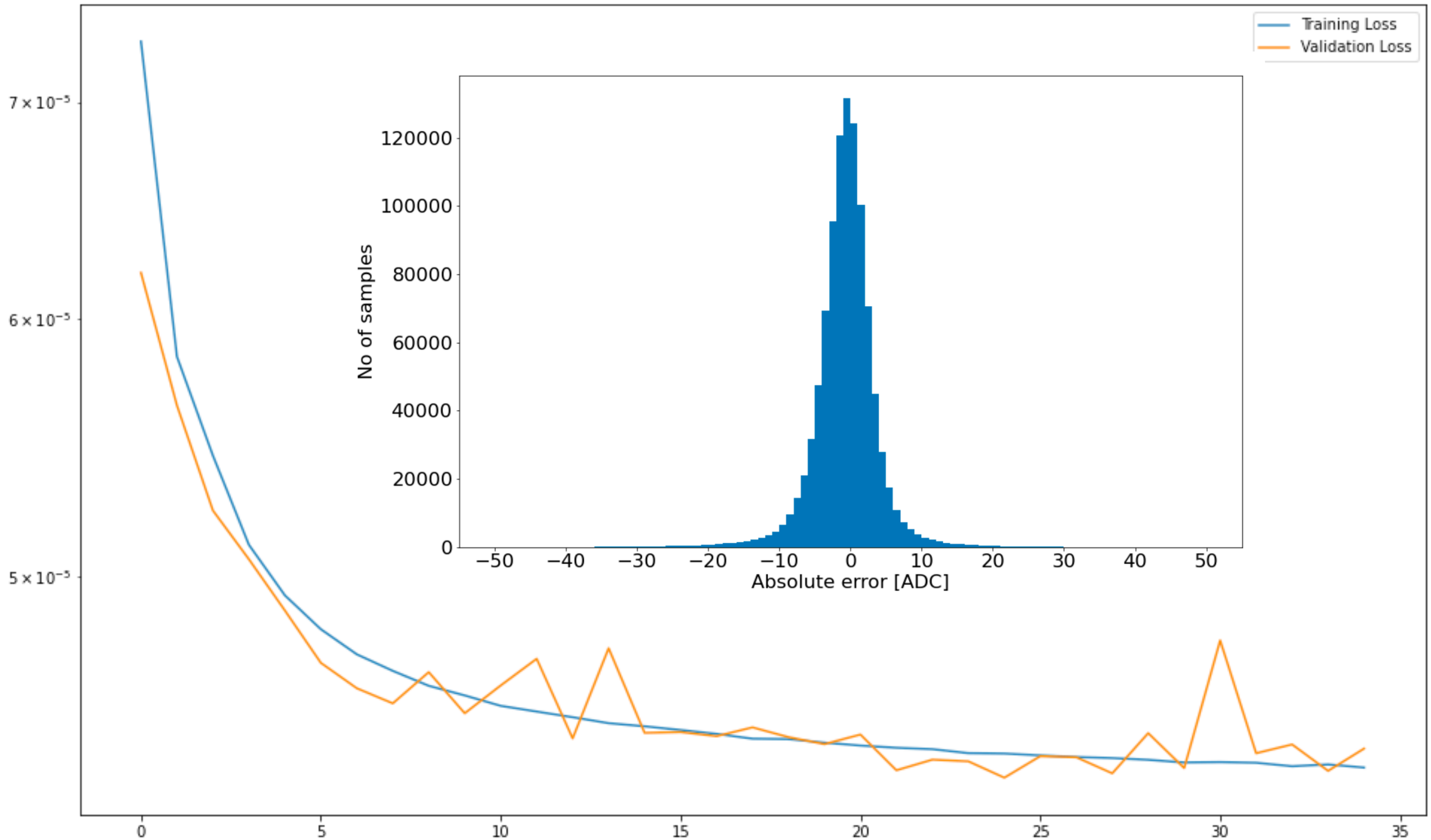


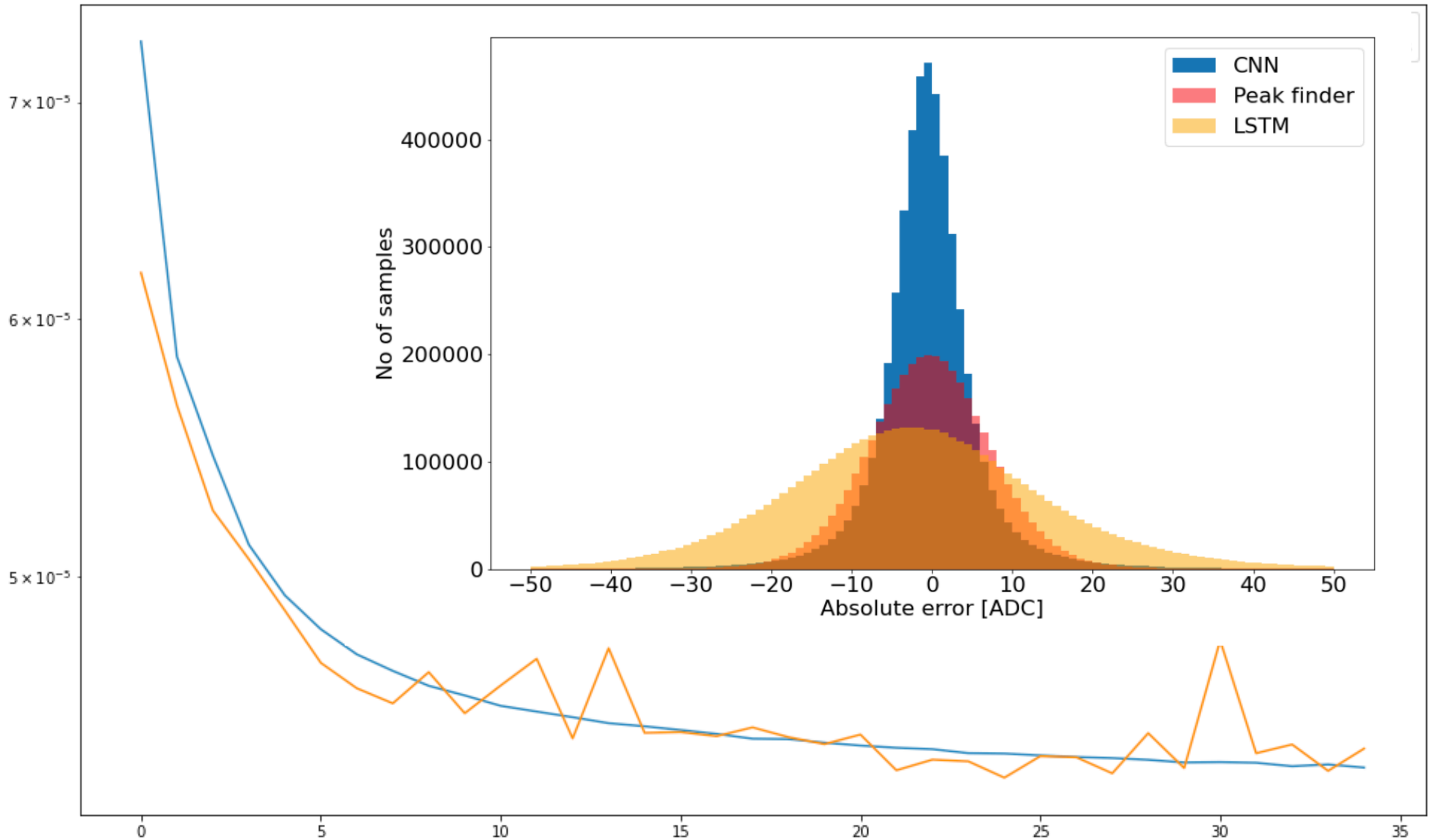



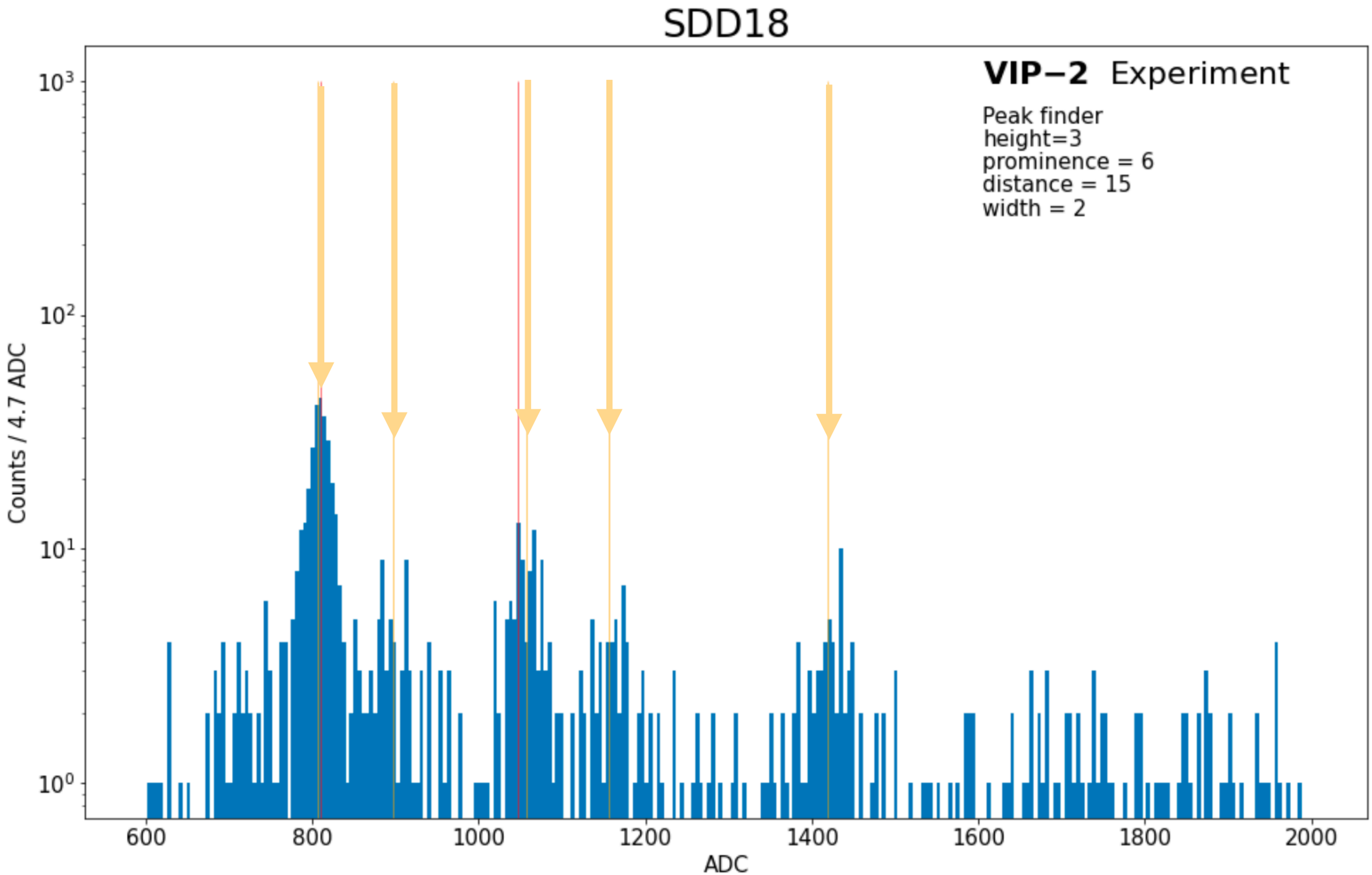

*Statistical fluctuations at low counts can make the use of peak finder algorithm tricky to setup needs constant care calibrated to be resilient algo params need to be tuned*

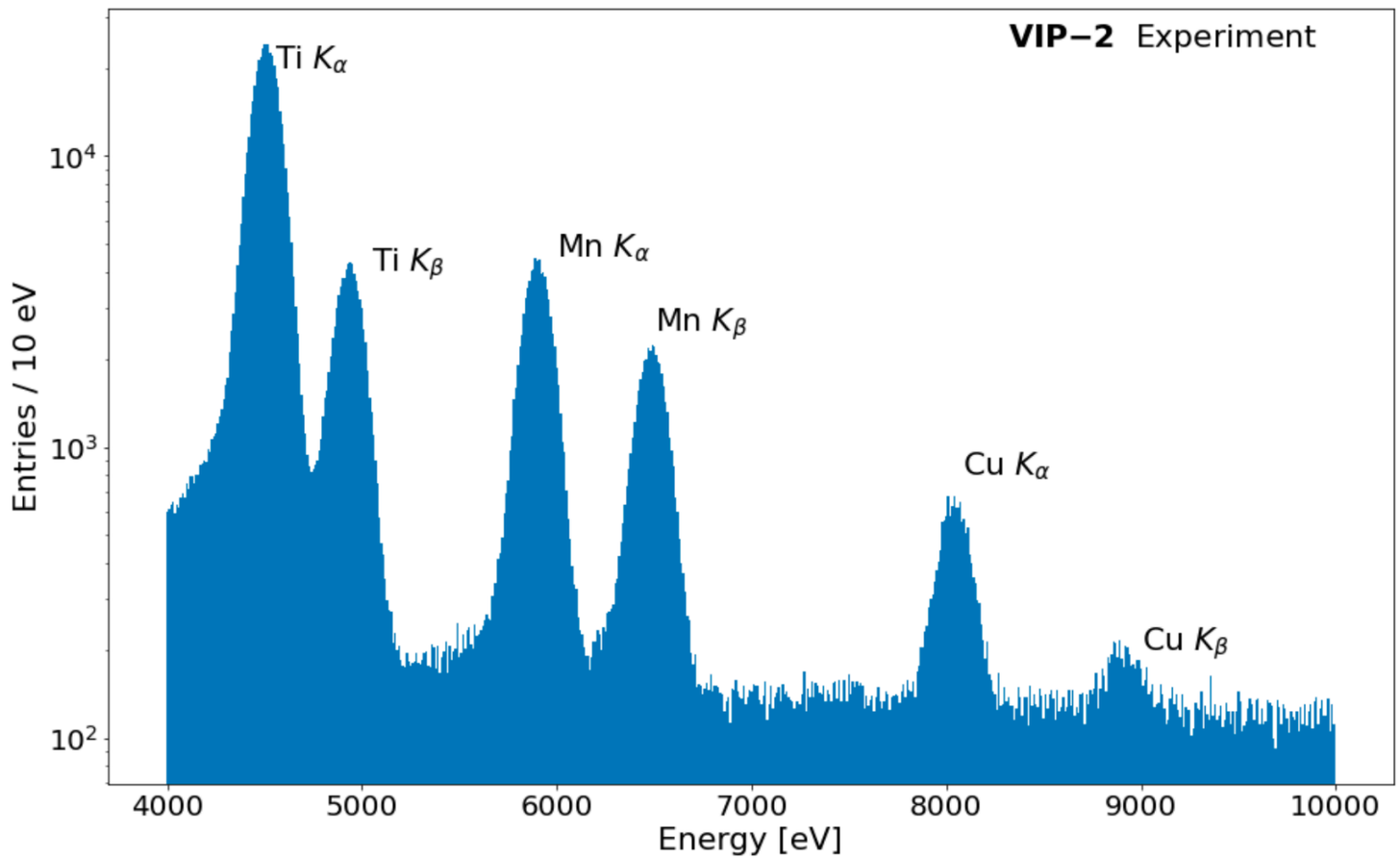
# Use two step approach - 1st: convolutional neural network as peak finder




CNN
Peak finder
LSTM
No of samples
Absolute error [ADC]
400000
300000
200000
100000
0
−50
−40
−30
−20
−10
0
10
20
30
40
50
7 × 10⁻⁵
6 × 10⁻⁵
5 × 10⁻⁵
0
5
10
15
20
25
30
35

*Use two step approach - 1st: convolutional neural network as peak finder*



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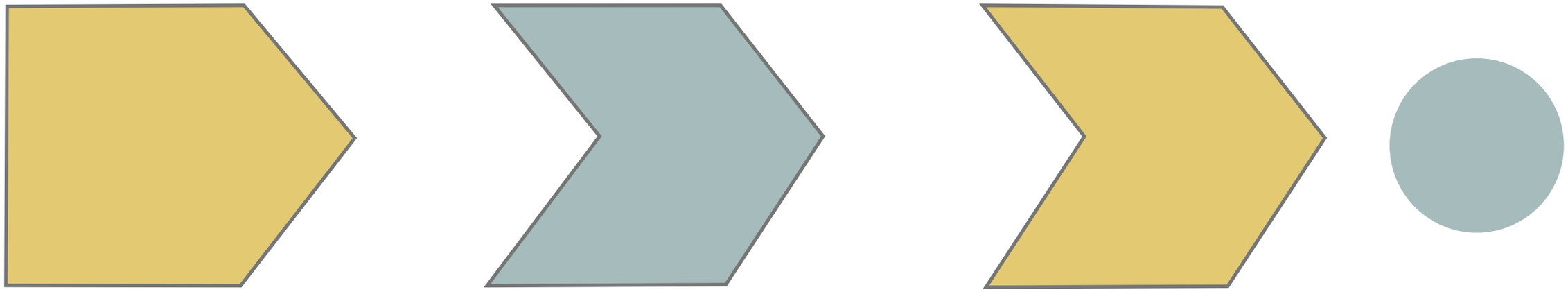
*Use two step approach - 2nd: to the limit with differentiable programming*



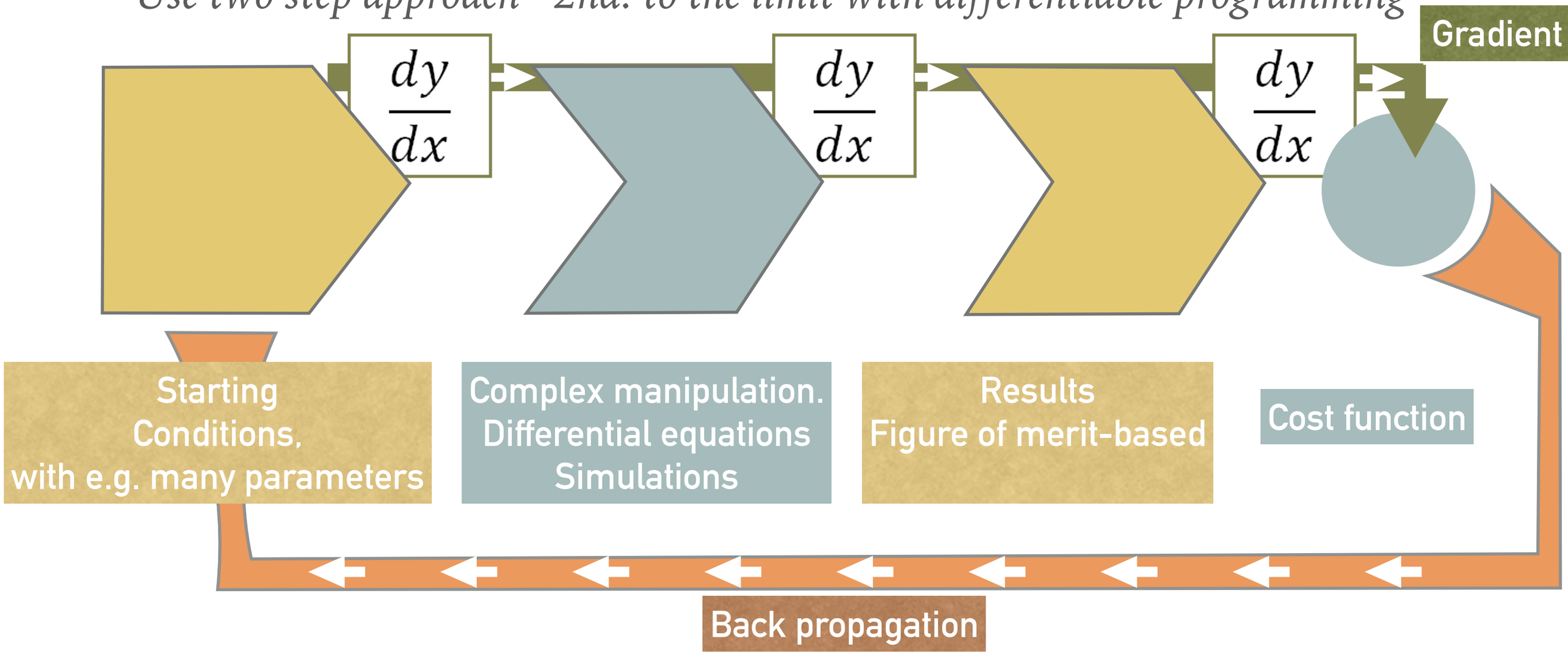
Starting Conditions, with e.g. many parameters

Complex manipulation. Differential equations Simulations

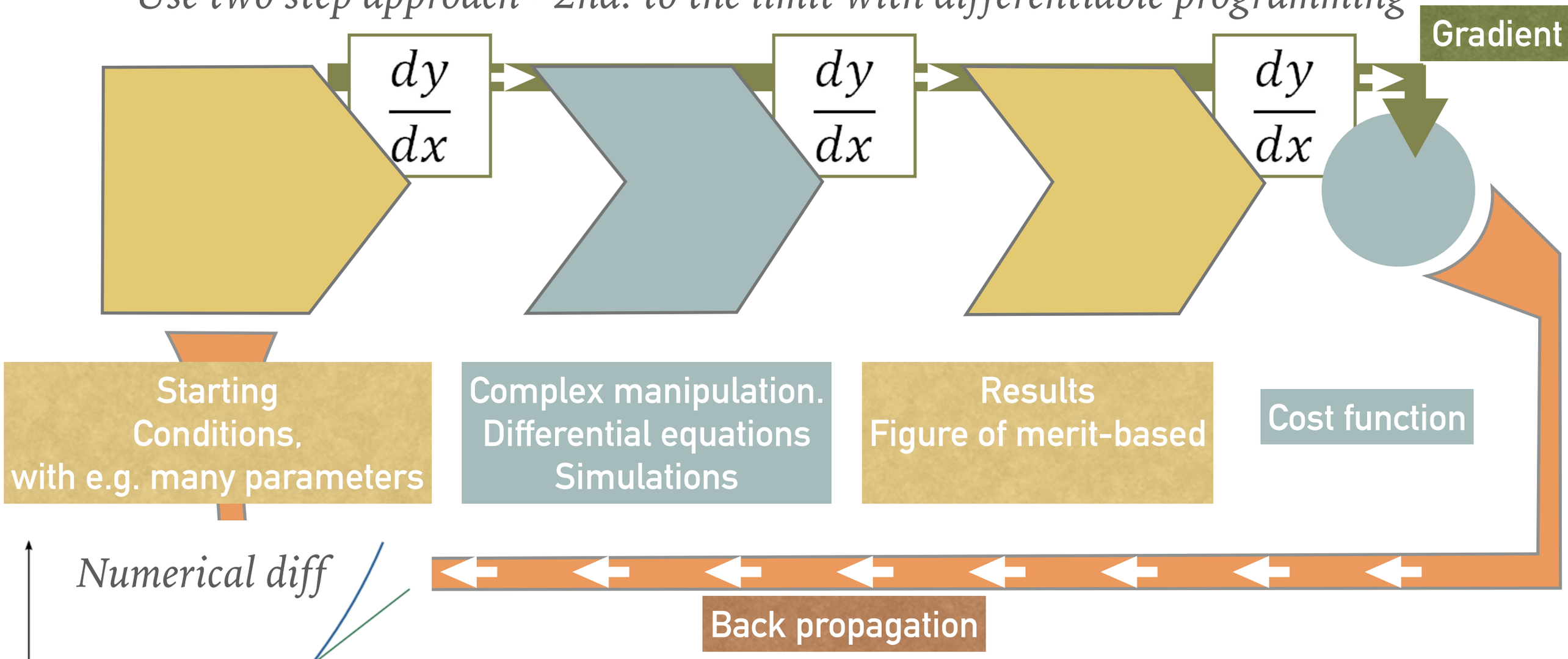
Results Figure of merit-based

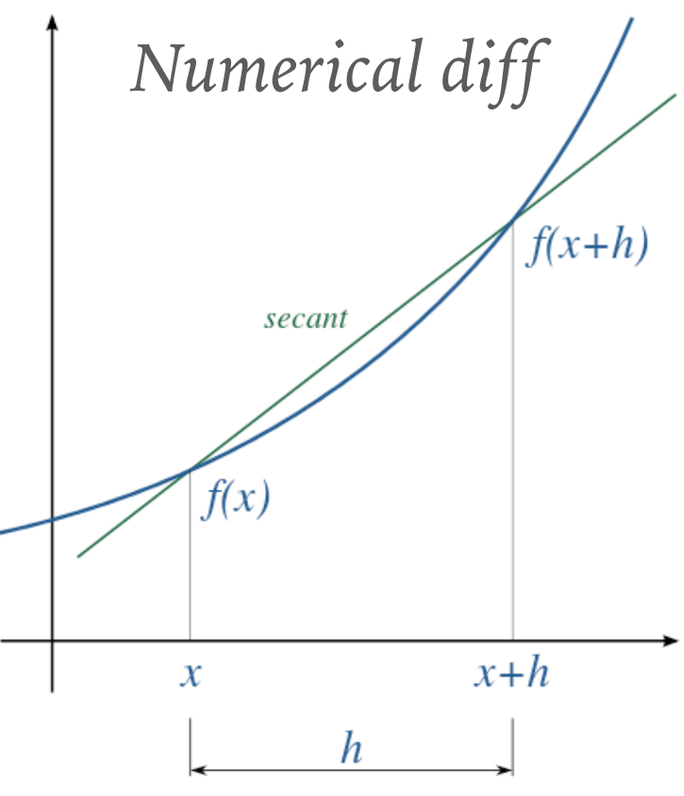
Cost function

*Use two step approach - 2nd: to the limit with differentiable programming*

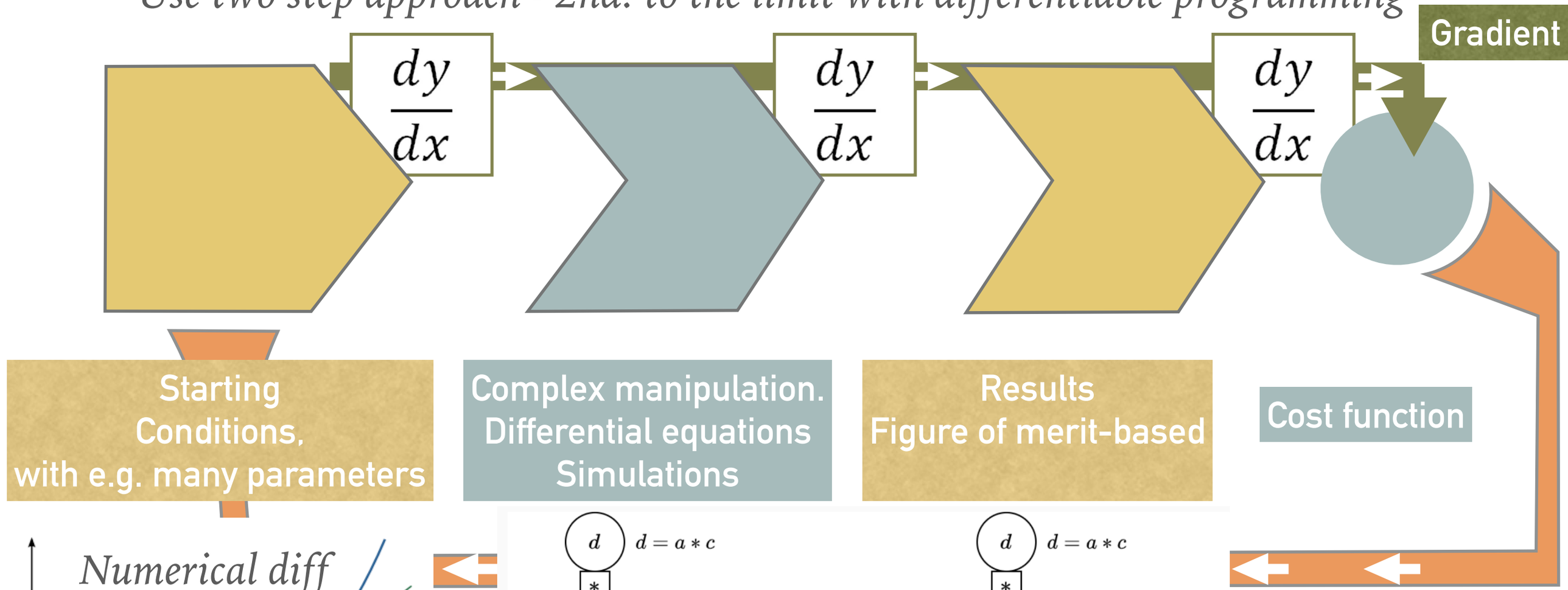


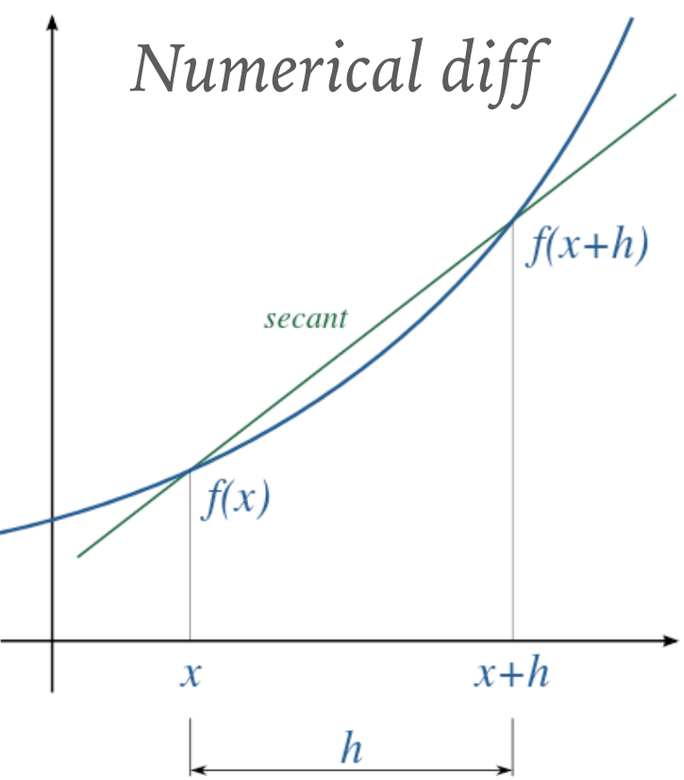
*Use two step approach - 2nd: to the limit with differentiable programming*

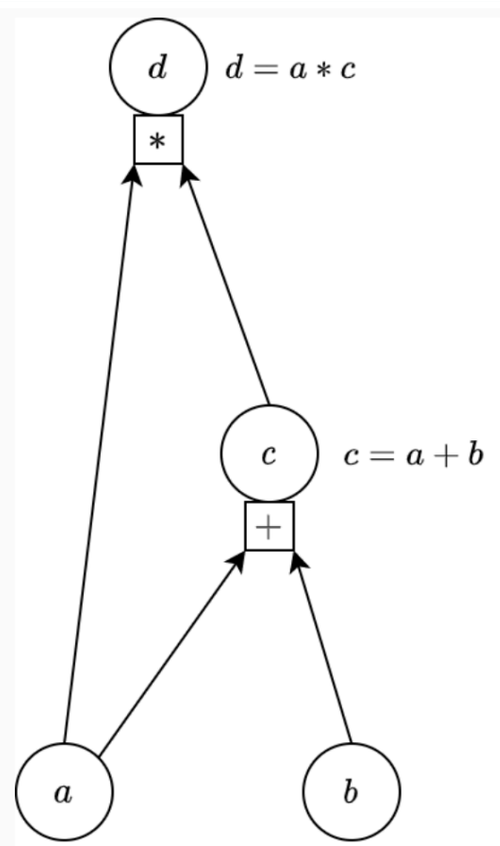


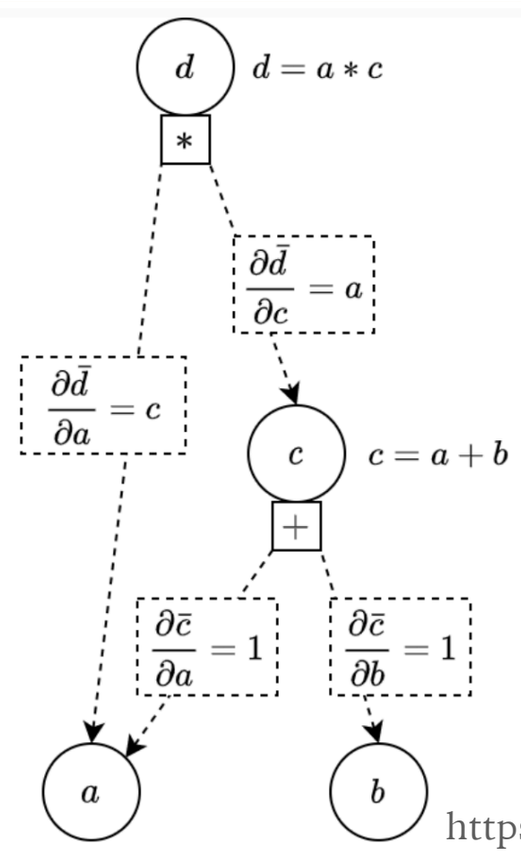



# Use two step approach - 2nd: to the limit with differentiable programming




$$\frac{\partial d}{\partial a} = \frac{\partial \bar{d}}{\partial a} + \frac{\partial \bar{d}}{\partial c} * \frac{\partial \bar{c}}{\partial a}$$

$$\frac{\partial d}{\partial a} = c + a * 1$$

$$\frac{\partial d}{\partial a} = a + b + a$$

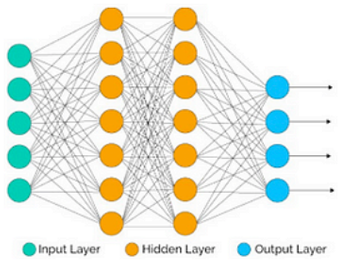
$$\frac{\partial d}{\partial a} = 2a + b$$

https://sidsite.com/posts/autodiff/

# Use two step approach - 2nd: to the limit with differentiable programming

Target and environment variables → Neural Network → Control Parameters → ODE Solver → Loss

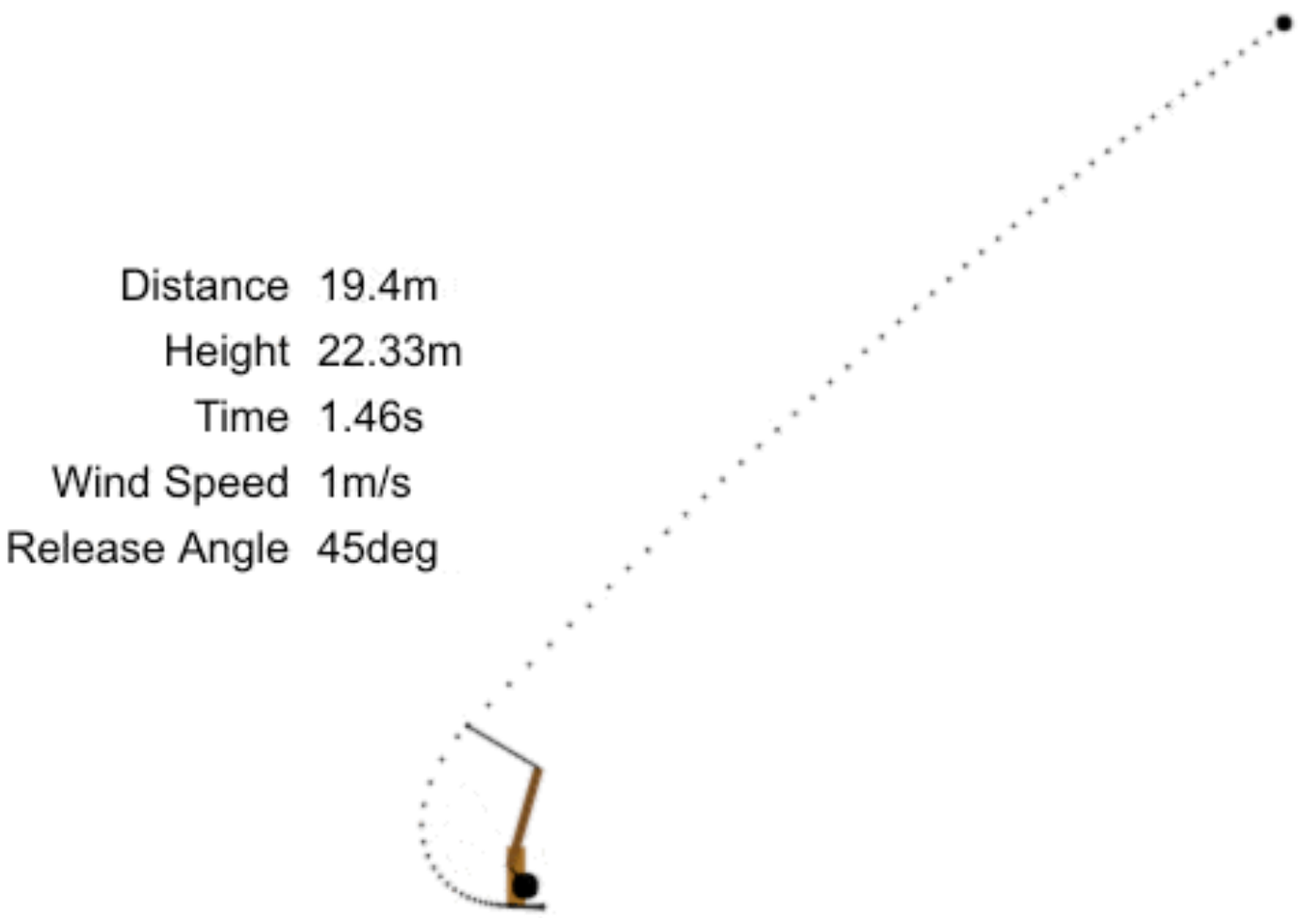
*wind = -10m/s*
*target = 50m*




*angle = 25°*
*weight = 200kg*

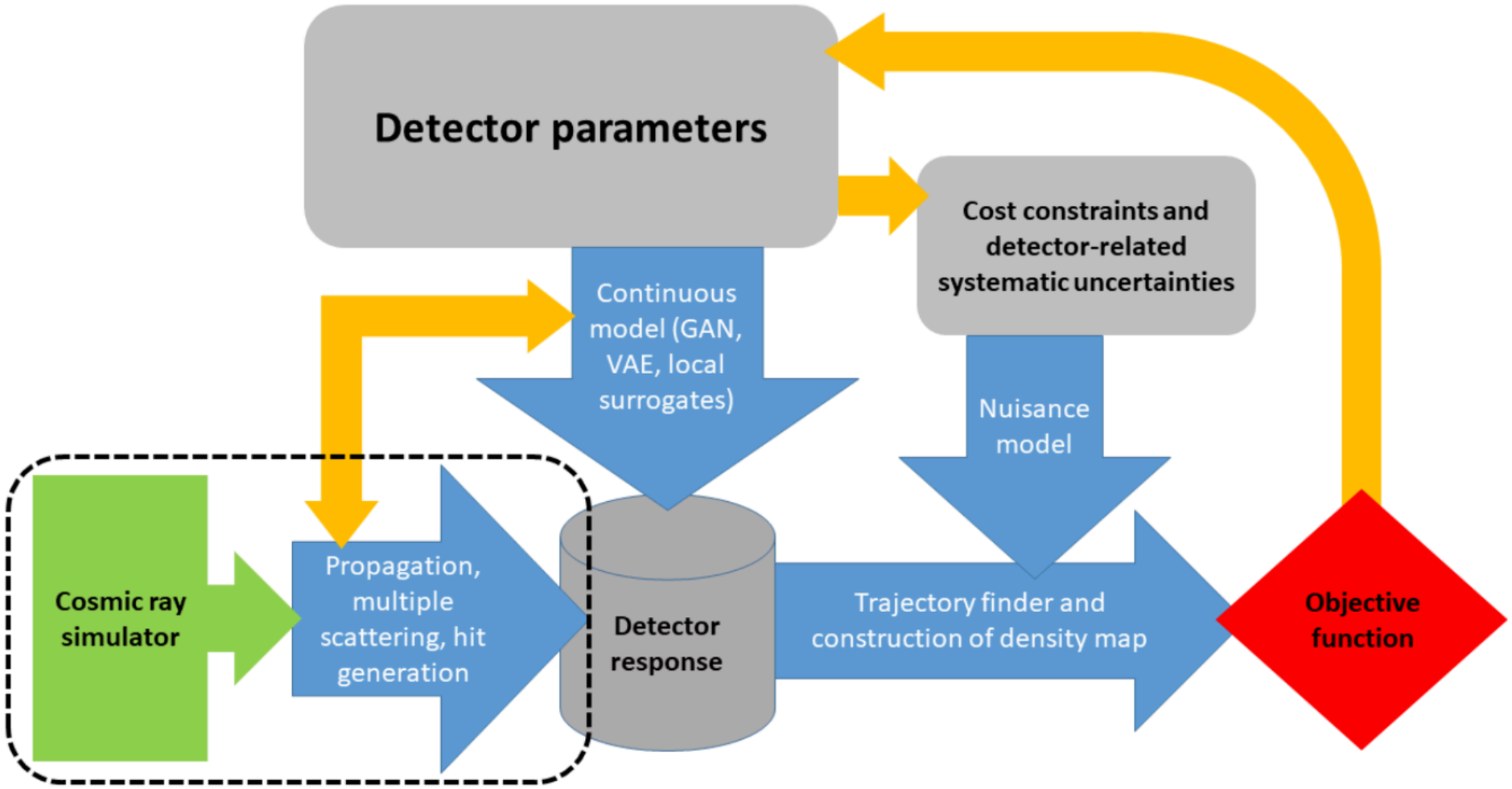
*(target_distance − actual_distance)²*

Backpropagation




https://github.com/JuliaComputing/ODSC2019

# Use two step approach - 2nd: to the limit with differentiable programming

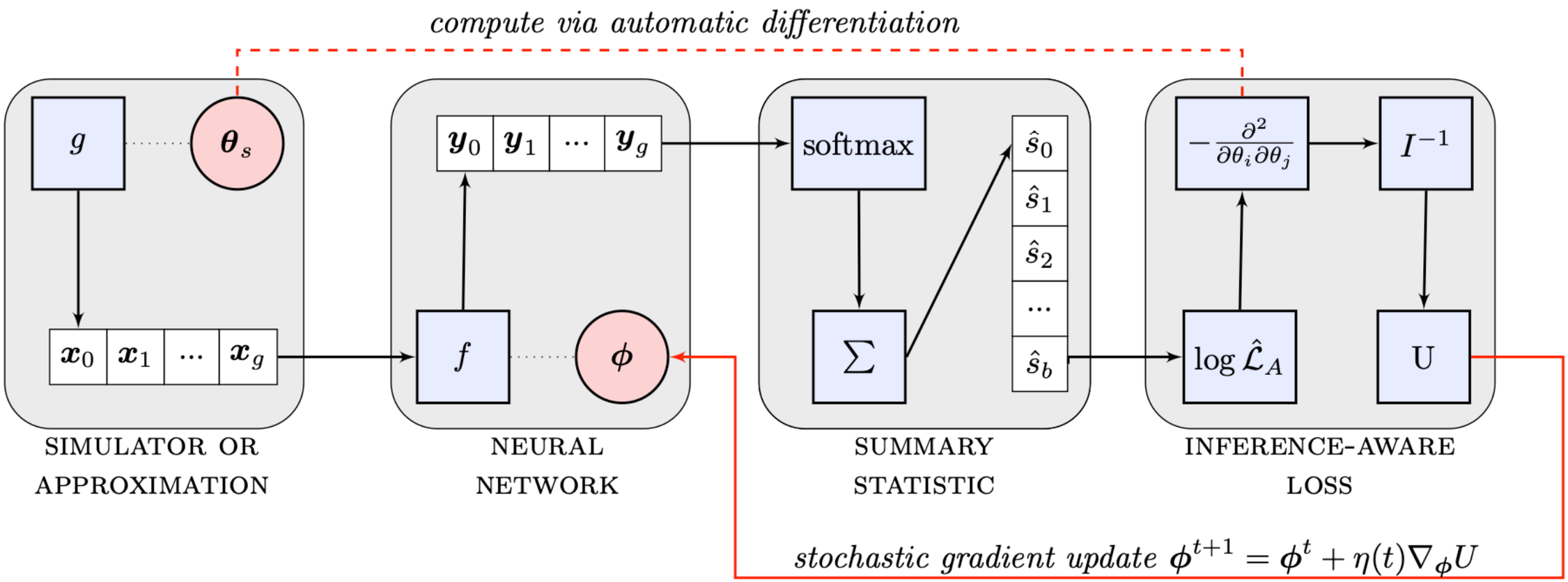



- *Optimization of detector design and operation*

MODE
Machine-learning Optimized Design of Experiments

https://inspirehep.net/files/8f6784eac6a7f06c184cfc50757de656

# Use two step approach - 2nd: to the limit with differentiable programming

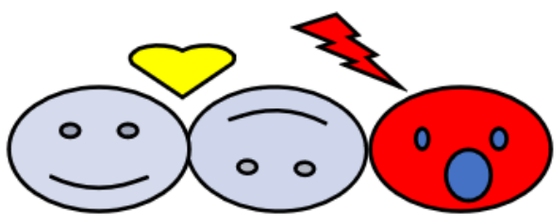



Sketch of the INFERNO algorithm. Batches from a simulator are passed through a neural network and a differentiable summary statistic is constructed that allows to calculate the variance of the POI. The parameters of the network are then updated by stochastic gradient descent.

https://cds.cern.ch/record/2807001/plots

# Use two step approach - 2nd: to the limit with differentiable programming

**Idea: use automatic differentiation to compute gradients of functions**
**Use gradients to find global optima**

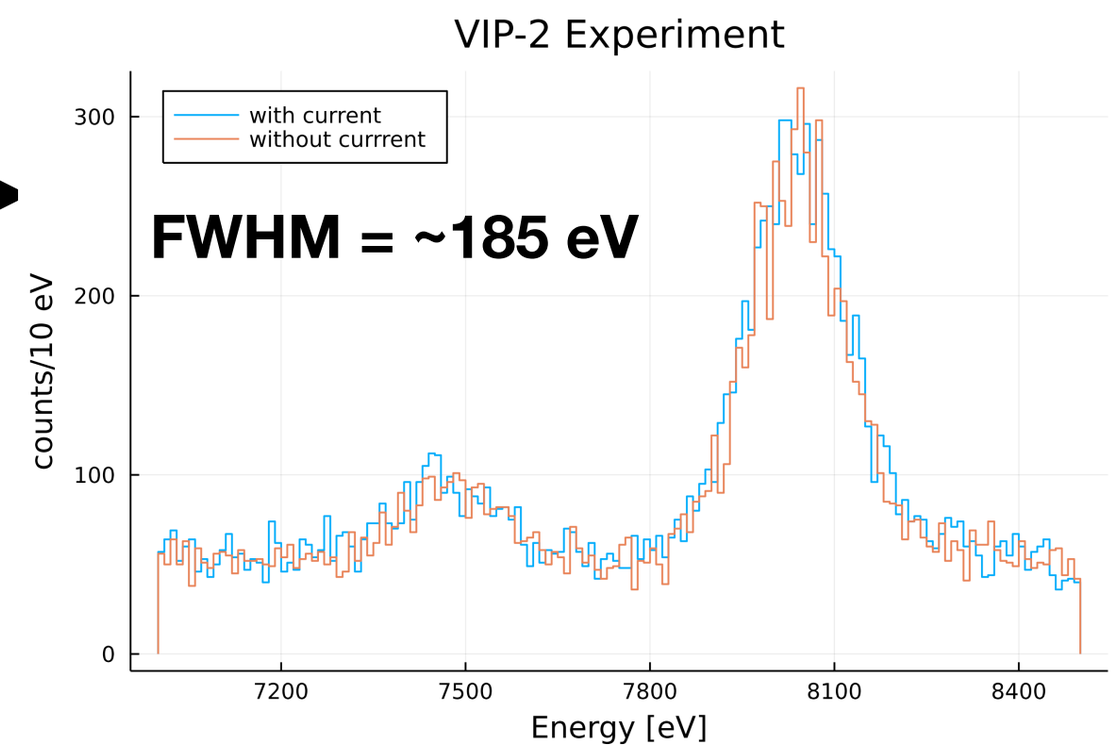


**Data**

**Fit peak positions**

**Derive calibration constants**

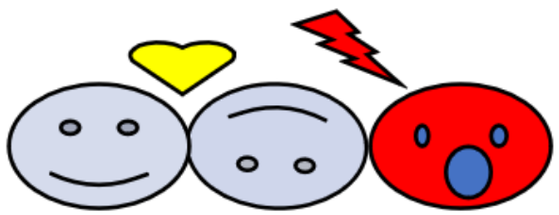
**Get calibrated data**




**Our Calibration Flow**

# Use two step approach - 2nd: to the limit with differentiable programming

**Idea: use automatic differentiation to compute gradients of functions**
**Use gradients to find global optima**



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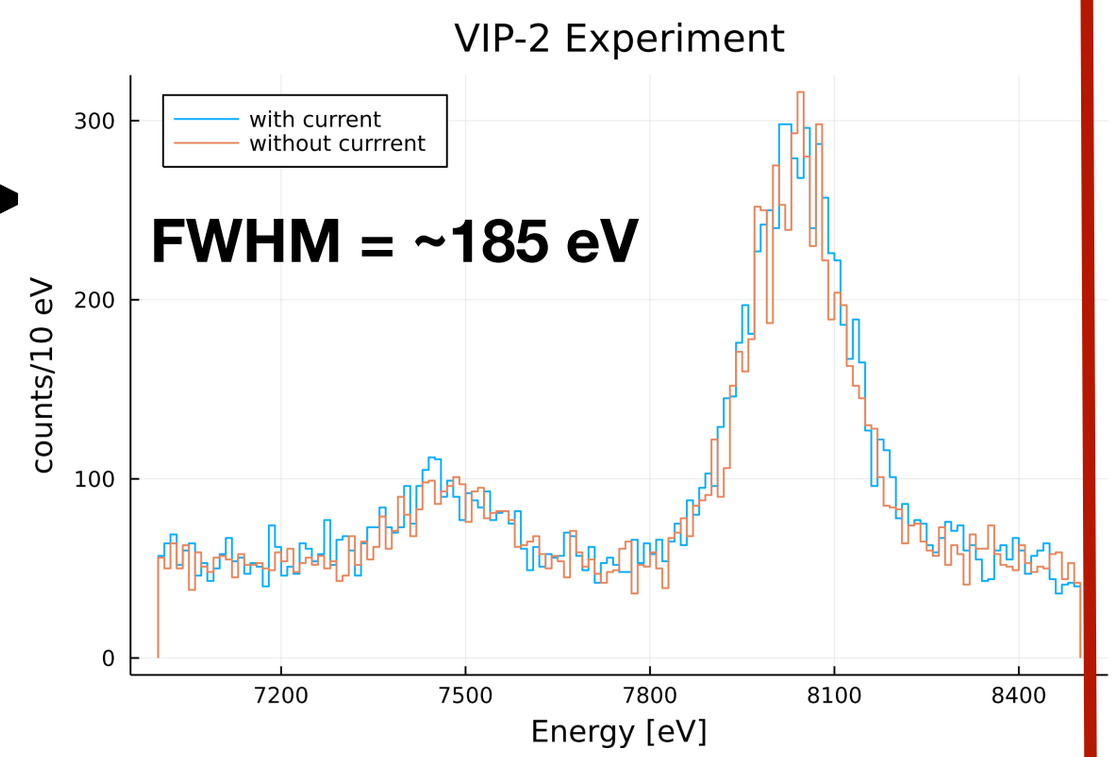
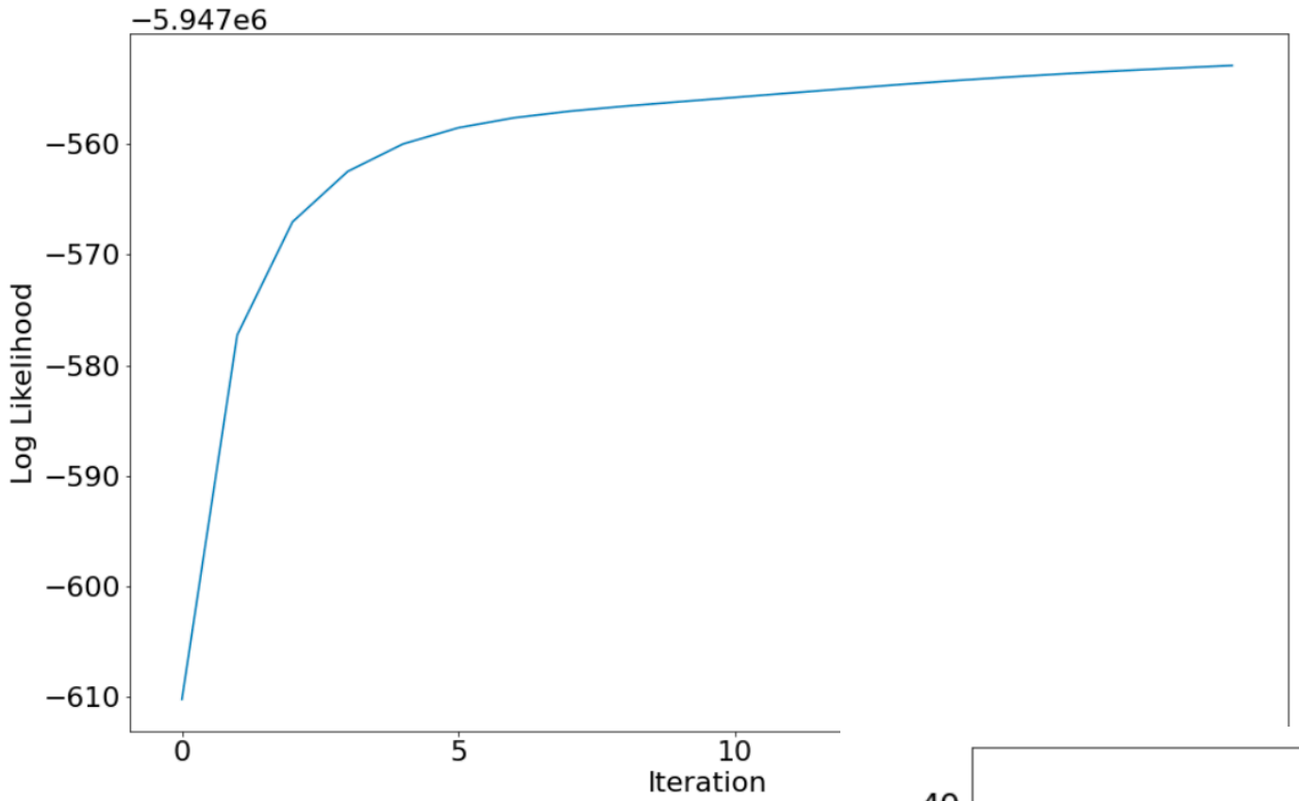


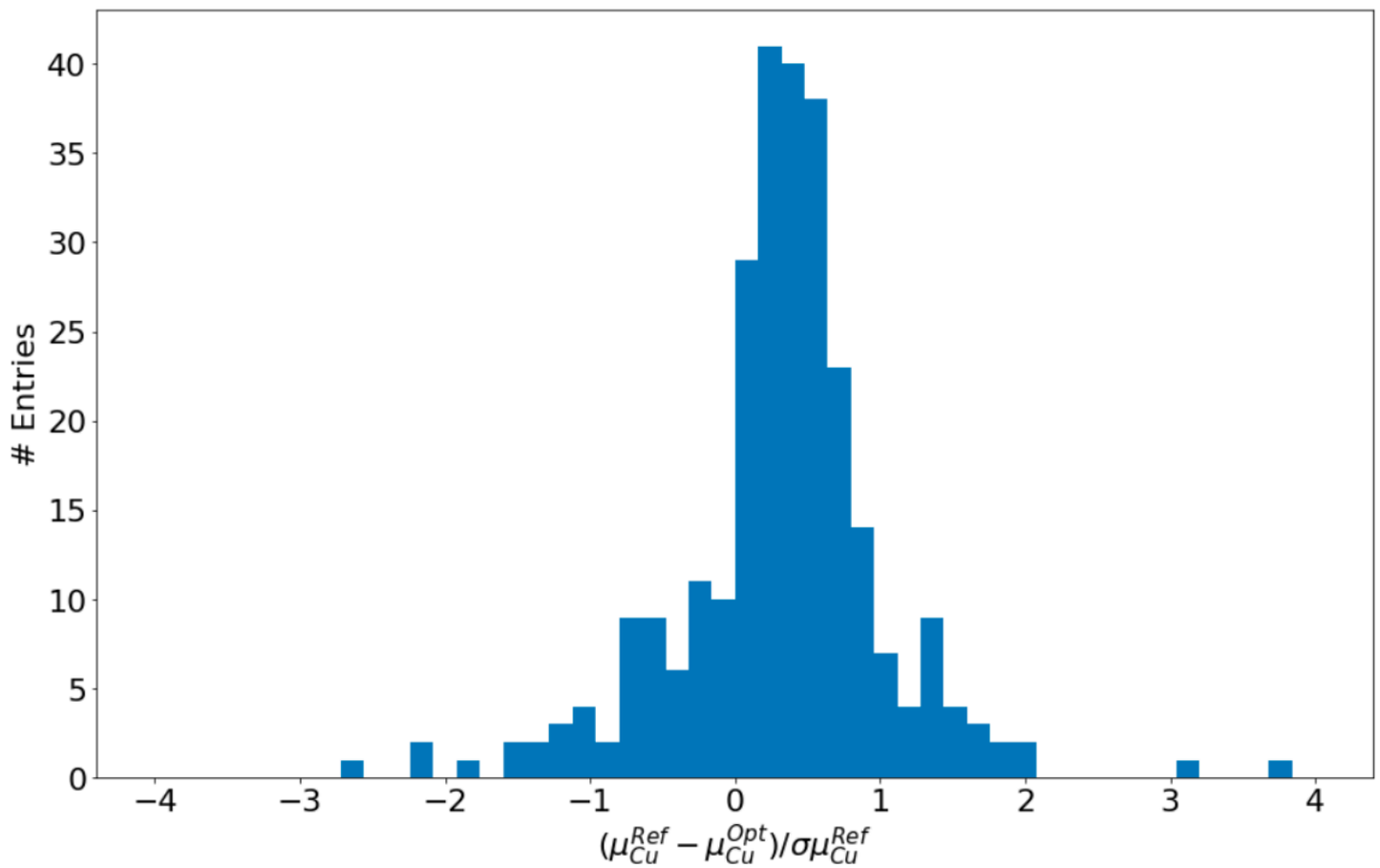

**Following the gradient, change the constants to enhance FWHM**

# Use two step approach - 2nd: to the limit with differentiable programming



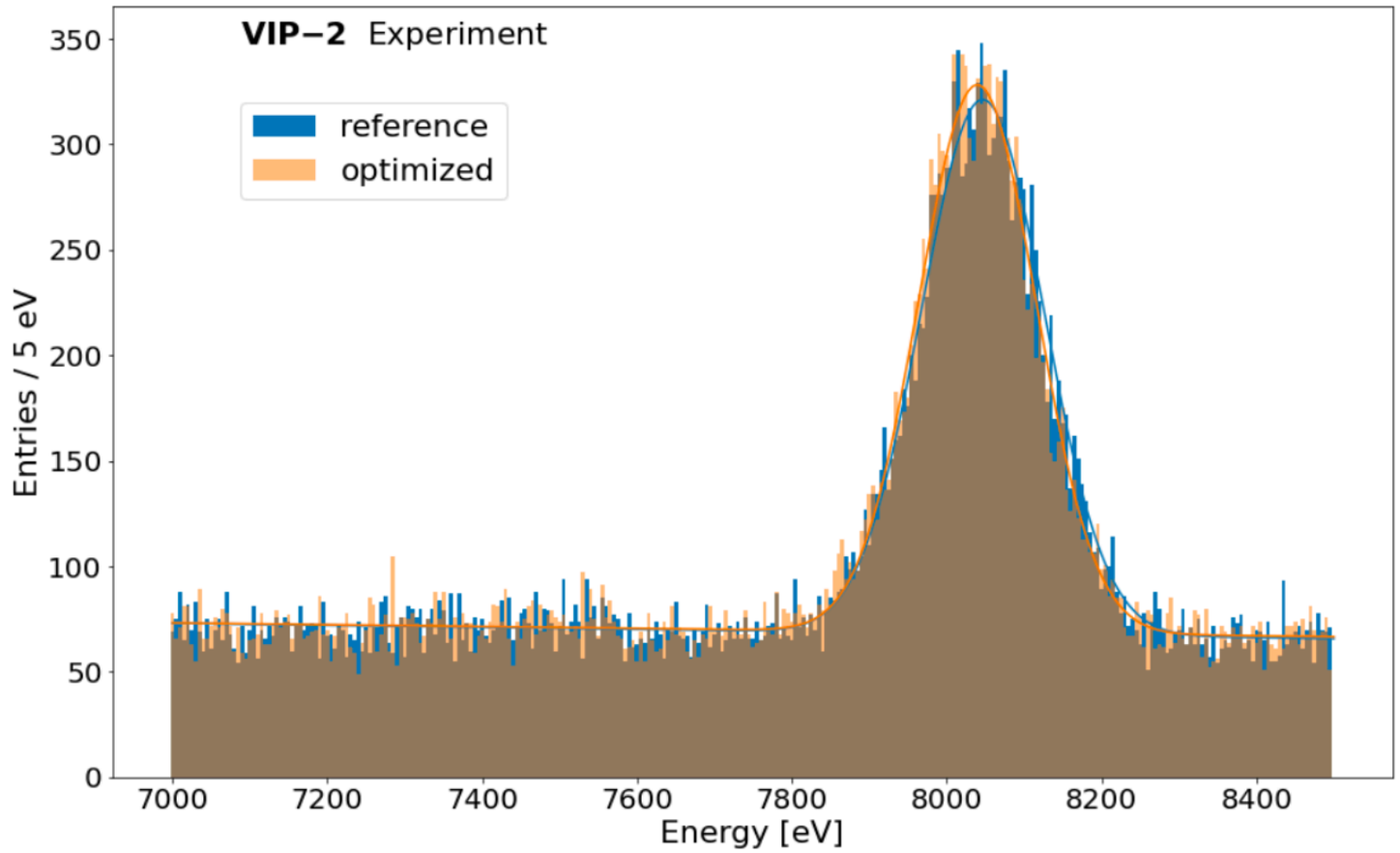

*Gradient descended into plateau*

*Most of the calibration parameters do not change much*



# Results

https://arxiv.org/abs/2305.17153
*Submitted to Meas. Sci. Tech.*




| | Position [eV] | FWHM [eV] | $\chi^2/ndf$ |
|---|---|---|---|
| Reference | $8050 \pm 1$ | $185 \pm 2$ | 1.64 |
| Optimized | $8048 \pm 1$ | $176 \pm 2$ | 1.25 |

$$f(x, A, \mu, \sigma) = A \times \frac{51}{100} \times \text{Gauss}(x-\mu-20, \sigma) + T_2(x) + A \times \text{Gauss}(x-\mu, \sigma) + T_1(x) + m \times x + C$$

$$T_i(x) = \frac{A_i}{2\beta\sigma} \times e^{\frac{x-\nu}{\beta\sigma}\frac{1}{2\beta^2}} \times erfc\left(\frac{x-\nu}{\sqrt{2}\pi} + \frac{1}{\sqrt{2}\beta}\right)$$