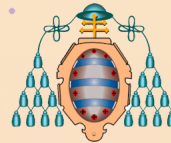


AI-assisted design of experiments at the frontiers of computation

methods and new perspectives

ICHEP 2024, Prague, Czech Republic

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vischia.github.io



UNIVERSIDAD DE OVIEDO



If you are reading this as a web page: have fun! If you are reading this as a PDF: please visit

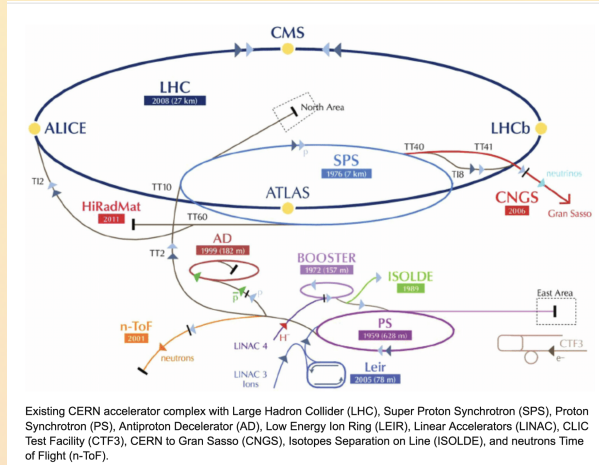
https://www.hep.uniovi.es/vischia/persistent/2024-07-20_AIAssistedDesignAfFrontiersOfComputationAtICHEP2024_vischia.html

to get the version with working animations

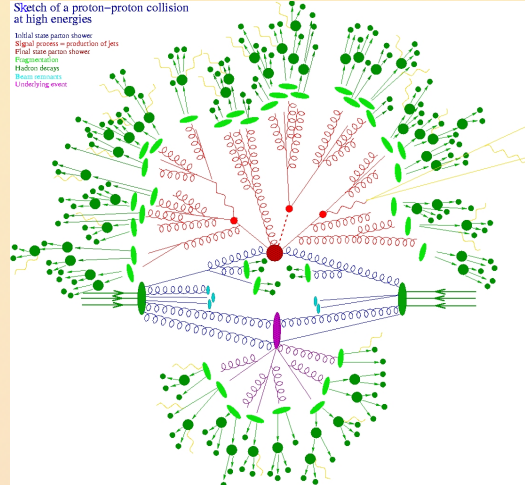
Complex experimental apparatusa

- 2020 European Strategy (EUSUPP): "New large, long-term projects, pushing technological skills to the limit"

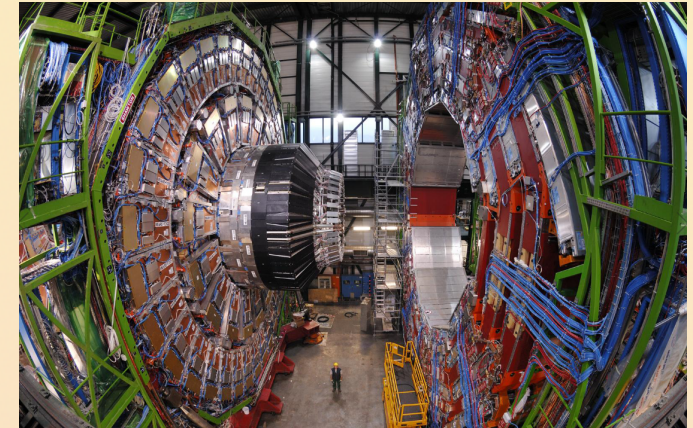
Complex accelerators



Complex phenomena



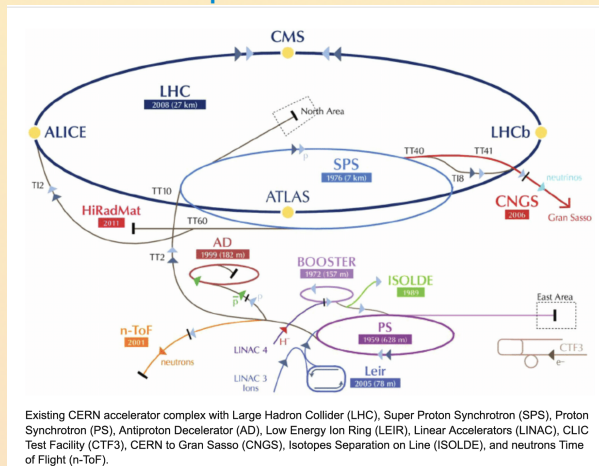
Complex experiments and reconstruction



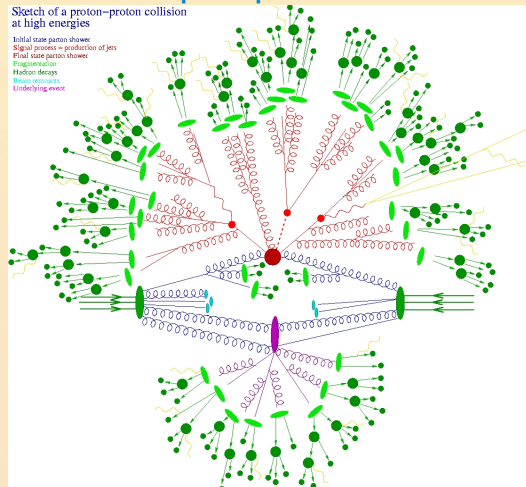
Complex experimental apparatusa

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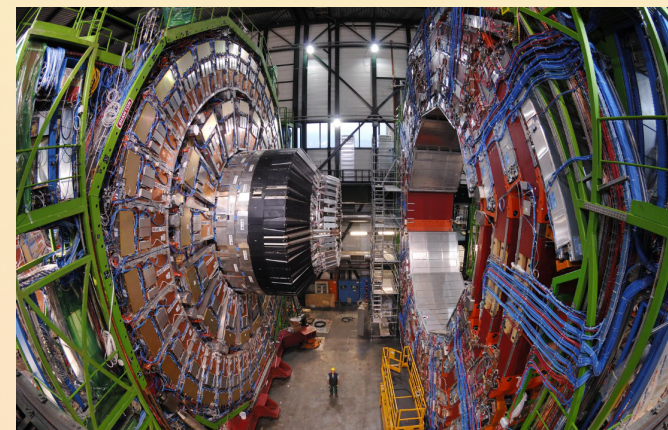
Complex accelerators



Complex phenomena



Complex experiments and reconstruction



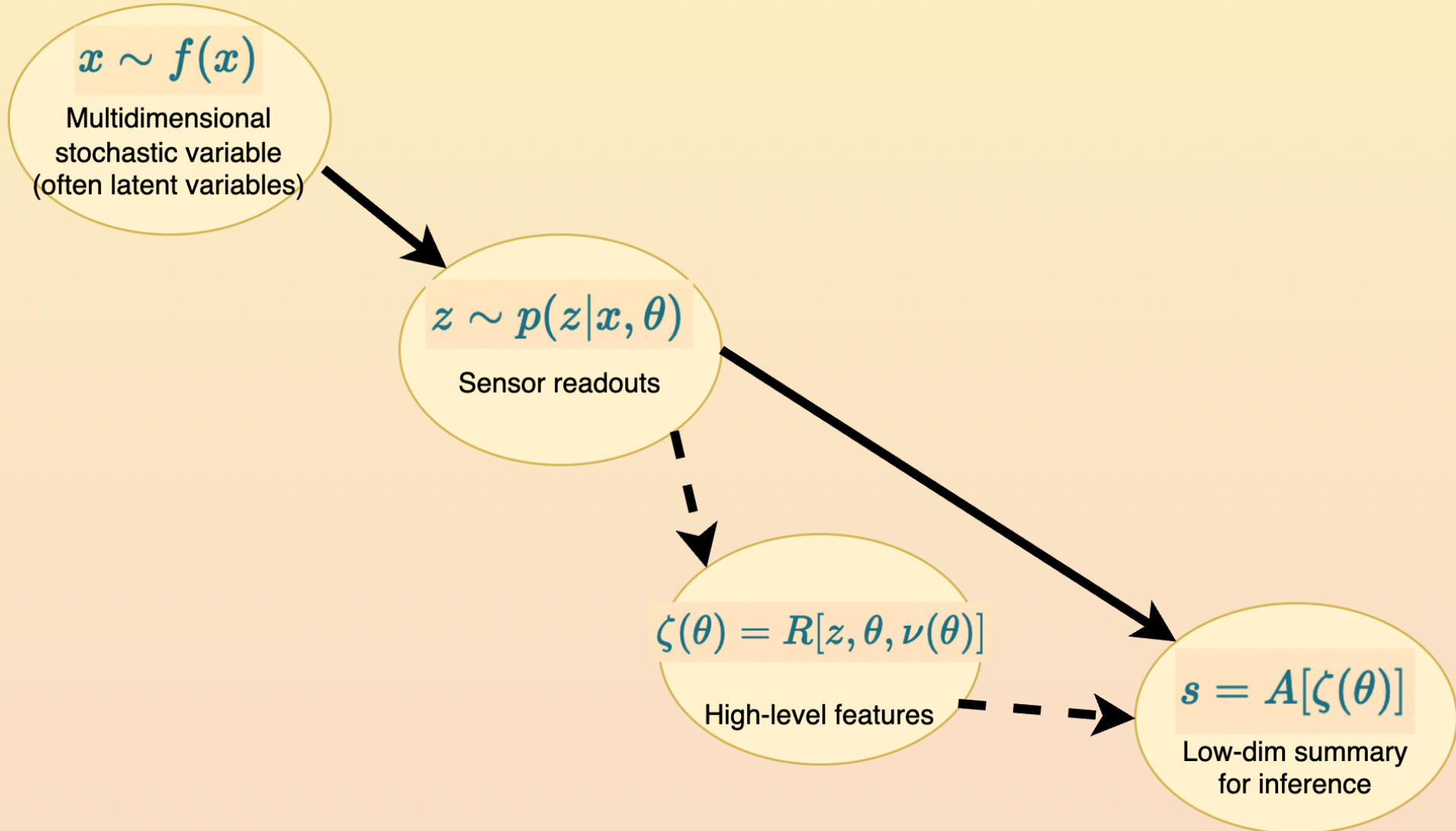
$$P(\mathbf{x}|\alpha) = \frac{1}{A_\alpha \sigma_\alpha} \int d\Phi(y) \frac{dx_1 dx_2}{x_1 x_2 s} f(x_1) f(x_2) |\mathcal{M}_\alpha(y, x_1, x_2)|^2 W(\mathbf{x}|y) \epsilon_\alpha(y)$$

Normalization factor
We collide protons and that is a mess
Linear operator in Hamiltonian formalism, describes the physics process
Detector response, experimental efficiencies

- Stochastic processes → intractable likelihood (matrix element, parton shower, detector simulation... result in latent variables)

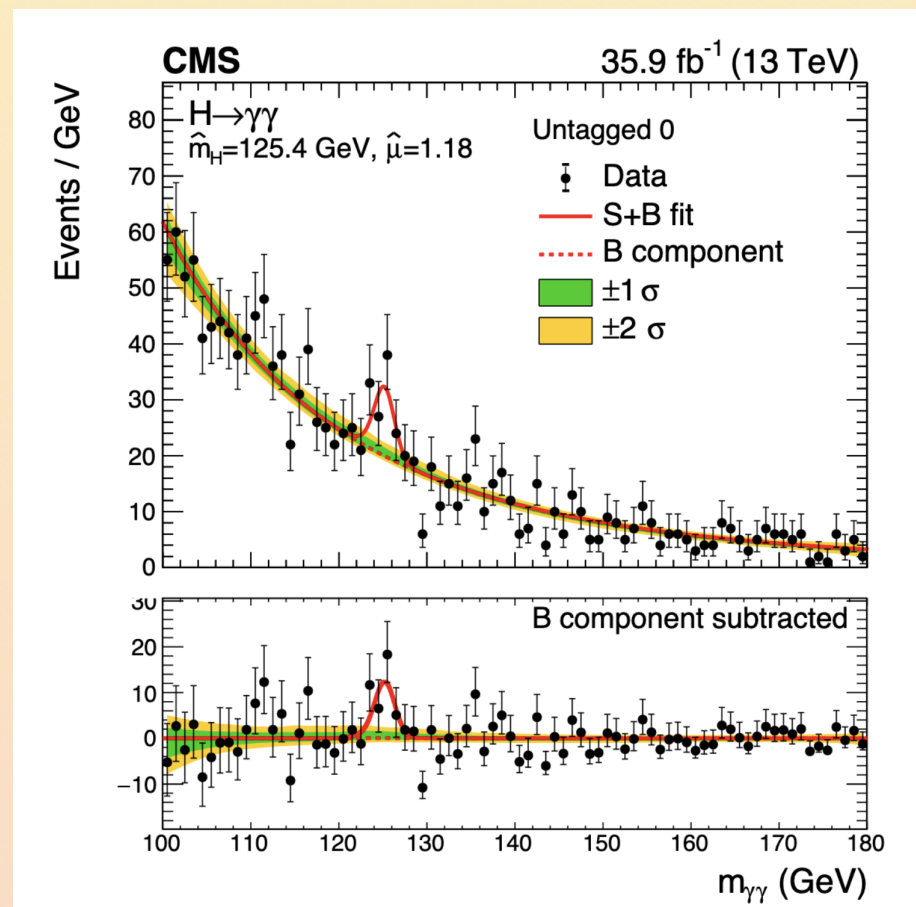
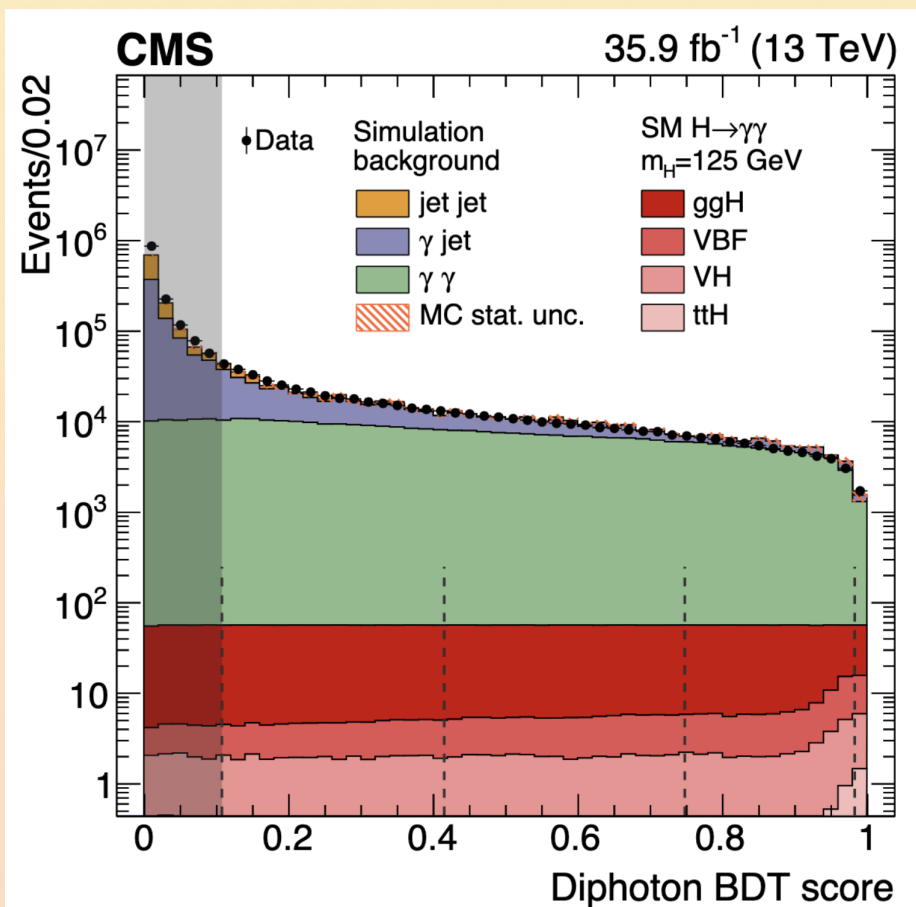
- Costly MonteCarlo simulators to generate $x \sim p(x|\theta)$ (for each event, several thousand randomized choices)

Typical analysis pipeline

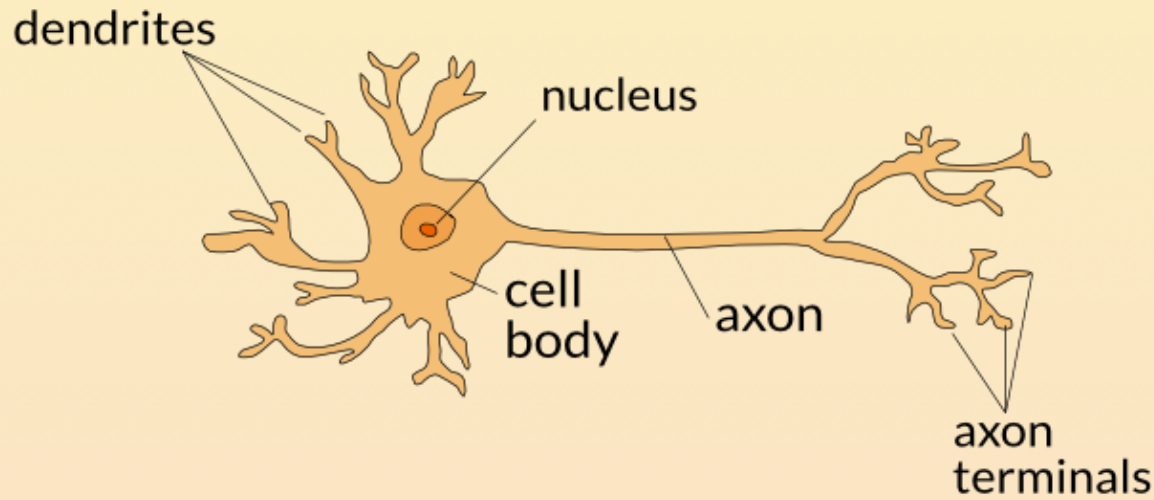


Can we go beyond histograms?

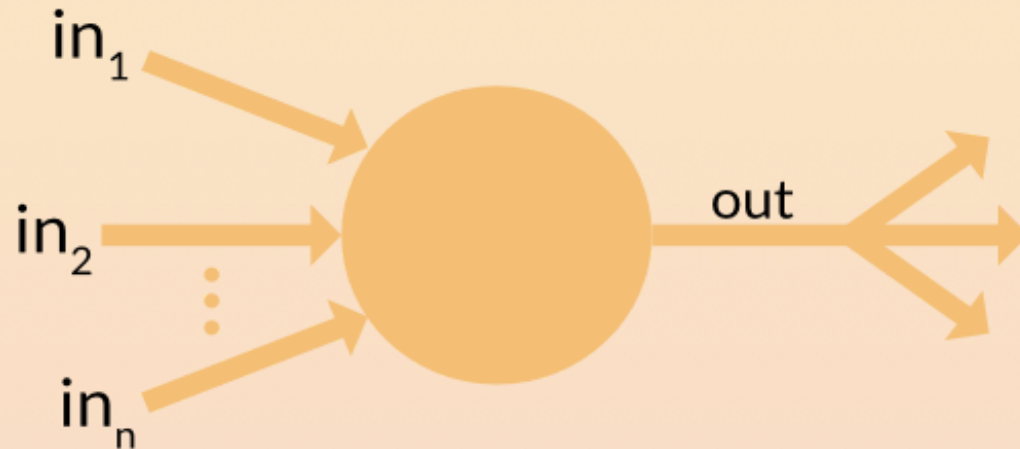
- Histograms are likelihood-free (count events, assume Poisson per bin, global likelihood as product)
- Can we optimize inference procedures through intractable problems?



From Neurons to Perceptrons



$$I(t) = C \frac{dV}{dt} + G_{Na} m^3 h (V - V_{Na}) + G_K n^4 (V - V_K) + G_L (V - V_L)$$

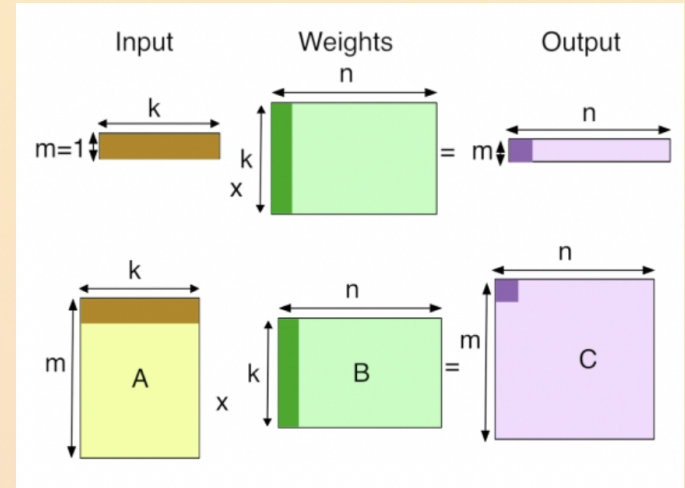
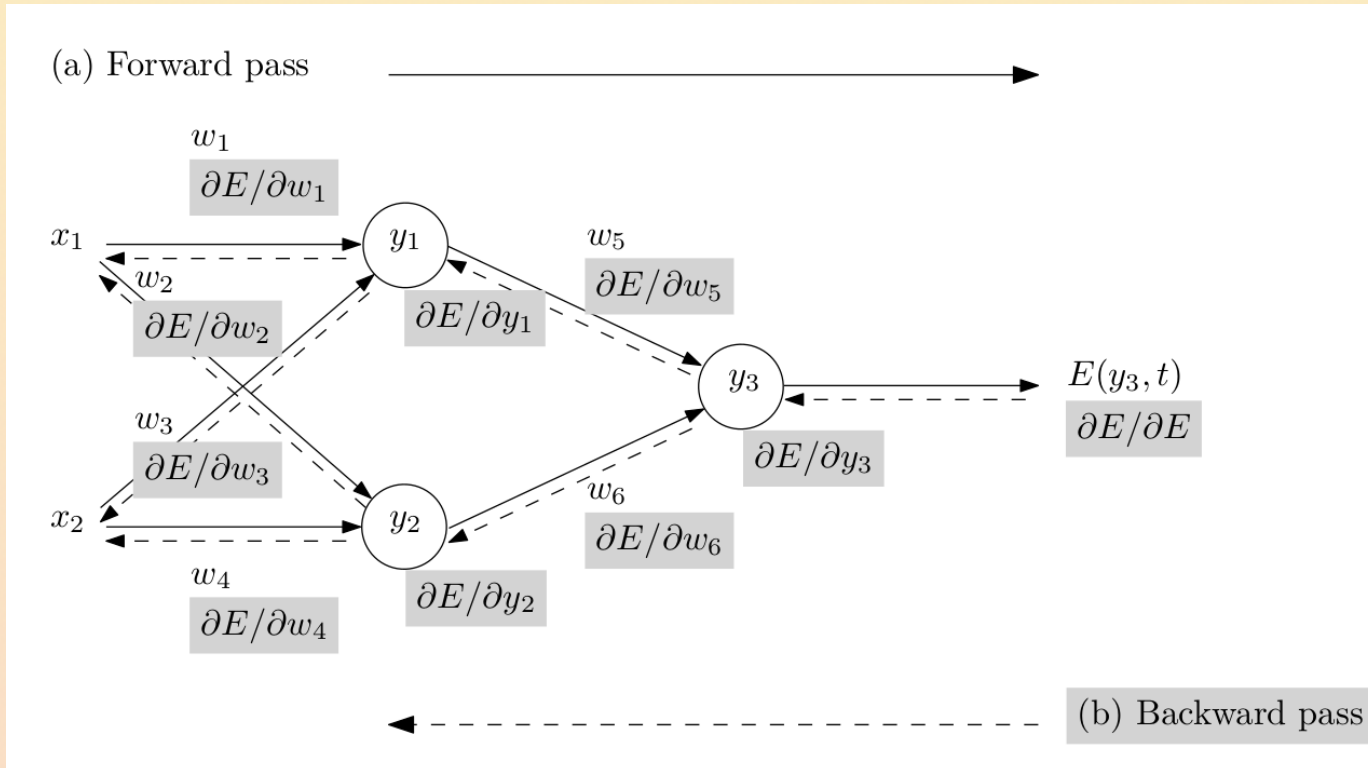


$$y = f\left(b_i + \sum w_i x_i\right)$$

Empirical Risk Minimization

$$\mathbf{J}(\mathbf{W}) = \frac{1}{n} \sum_{i=1}^n \mathcal{L}(f(x^{(i)}; \mathbf{W}), y^{*(i)}), \quad \mathbf{W}^0 = \operatorname{argmin}_{\mathbf{W}} \mathbf{J}(\mathbf{W}), \quad \mathbf{W} \leftarrow \mathbf{W} + \eta \frac{\partial \mathbf{J}(\mathbf{W})}{\partial \mathbf{W}}$$

- Efficient matrix multiplication in dedicated hardware (GPUs, FPGAs)



Autodiff powers most of modern ML

- By design, simple in software

```
import torch, math
x0 = torch.tensor(1., requires_grad=True)
x1 = torch.tensor(2., requires_grad=True)
p = 2*x0 + x0*torch.sin(x1) + x1**3
print(p)
p.backward()
print(x0.grad, x1.grad)
```

yielding

```
Primal: tensor(10.9093, grad_fn=<AddBackward0>)
Adjoint: tensor(2.9093) tensor(11.5839)
```

- Computational cost of calculating $\mathbf{J}_f(\mathbf{x})$ in $\mathbb{R}^n \times \mathbb{R}^m$ for $f: \mathbb{R}^n \rightarrow \mathbb{R}^m$
 - $\mathcal{O}(n \text{ time}(f))$
 - $\mathcal{O}(m \text{ time}(f))$

$$y(\mathbf{x}) = 2x_0 + x_0 \sin(x_1) + x_1^3$$

<i>Fwd Primal Trace Atomic operation</i>	<i>Value in (1, 2)</i>	<i>Fwd Tangent Trace (set $\dot{x}_0 = 1$ to compute $\frac{\partial y}{\partial x_0}$) Atomic operation</i>	<i>Value in (1, 2)</i>
$v_0 = x_0$ $v_1 = x_1$	1 2	$\dot{v}_0 = \dot{x}_0$ $\dot{v}_1 = \dot{x}_1$	1 0
$v_2 = 2v_0$ $v_3 = \sin(v_1)$ $v_4 = v_0 v_3$ $v_5 = v_1^3$ $v_6 = v_2 + v_4 + v_5$	2 0.9093 0.9093 8 10.9093	$\dot{v}_2 = 2\dot{v}_0$ $\dot{v}_3 = \dot{v}_1 \cos(v_1)$ $\dot{v}_4 = \dot{v}_0 v_3 + v_0 \dot{v}_3$ $\dot{v}_5 = 3\dot{v}_1 v_1^2$ $\dot{v}_6 = \dot{v}_2 + \dot{v}_4 + \dot{v}_5$	2×1 0×-0.41 $1 \times 0.9093 + 1 \times 0$ 0 $3 \times 0 \times 4$ $2 + 0.9093 + 0$
$y = v_6$	10.9093	$\dot{y} = \dot{v}_6$	2.9093

<i>Fwd Primal Trace Atomic operation</i>	<i>Value in (1, 2)</i>	<i>Rev Adjoint Trace (set $\bar{y} = 1$ to compute $\frac{\partial v}{\partial y}$) Atomic operation</i>	<i>Value in (1, 2)</i>
$v_0 = x_0$ $v_1 = x_1$	1 2	$\bar{x}_0 = \bar{v}_0$ $\bar{x}_1 = \bar{v}_1$	2.9093 11.5839
$v_2 = 2v_0$ $v_3 = \sin(v_1)$ $v_4 = v_0 v_3$ $v_5 = v_1^3$ $v_6 = v_2 + v_4 + v_5$	2 0.9093 0.9093 8 10.9093	$\bar{v}_0 = \bar{v}_0 + \bar{v}_2 \partial v_2 / \partial v_0$ $\bar{v}_0 = \bar{v}_4 \partial v_4 / \partial v_0$ $\bar{v}_1 = \bar{v}_1 + \bar{v}_3 \partial v_3 / \partial v_1$ $\bar{v}_1 = \bar{v}_5 \partial v_5 / \partial v_1$ $\bar{v}_2 = \bar{v}_6 \partial v_6 / \partial v_2$ $\bar{v}_3 = \bar{v}_4 \partial v_4 / \partial v_3$ $\bar{v}_4 = \bar{v}_6 \partial v_6 / \partial v_4$ $\bar{v}_5 = \bar{v}_6 \partial v_6 / \partial v_5$	$\bar{v}_0 + \bar{v}_2 \times 2 = 2.9093$ $\bar{v}_4 \times v_3 = 0.9093$ $\bar{v}_1 + \bar{v}_3 \times \cos(v_1) = 11.5839$ $\bar{v}_5 \times 3v_1^2 = 12$ $\bar{v}_6 \times 1 = 1$ $\bar{v}_4 \times v_0 = 1$ $\bar{v}_6 \times 1 = 1$ $\bar{v}_6 \times 1 = 1$
$y = v_6$	10.9093	$\bar{v}_6 = \bar{y}$	1

Differentiable Programming

Execute **differentiable functions**
(programs)
via **automatic differentiation**



Yann LeCun ✓

January 5, 2018 · 🌐

OK, Deep Learning has outlived its usefulness as a buzz-phrase.

Deep Learning est mort. Vive Differentiable Programming!

Yeah, Differentiable Programming is little more than a **rebranding** of the modern collection Deep Learning techniques, the same way Deep Learning was a rebranding of the modern incarnations of neural nets with more than two layers.

But the important point is that people are now **building a new kind of software** by assembling networks of parameterized functional blocks and by training them from examples using some form of gradient-based optimization.

An increasingly large number of people are defining the networks procedurally in a data-dependent way (with loops and conditionals), allowing them to change dynamically as a function of the **input data fed to them**. It's really very much like a regular program, except it's parameterized, **automatically differentiated**, and trainable/optimizable. Dynamic networks have **become** increasingly popular (particularly for NLP), thanks to deep learning frameworks that can handle them such as PyTorch and Chainer (note: our old deep learning framework Lush could handle a particular kind of dynamic nets called Graph Transformer Networks, back in 1994. It was needed for text recognition).

People are now actively working on compilers for **imperative differentiable programming languages**. This is a very exciting avenue for the development of learning-based AI.

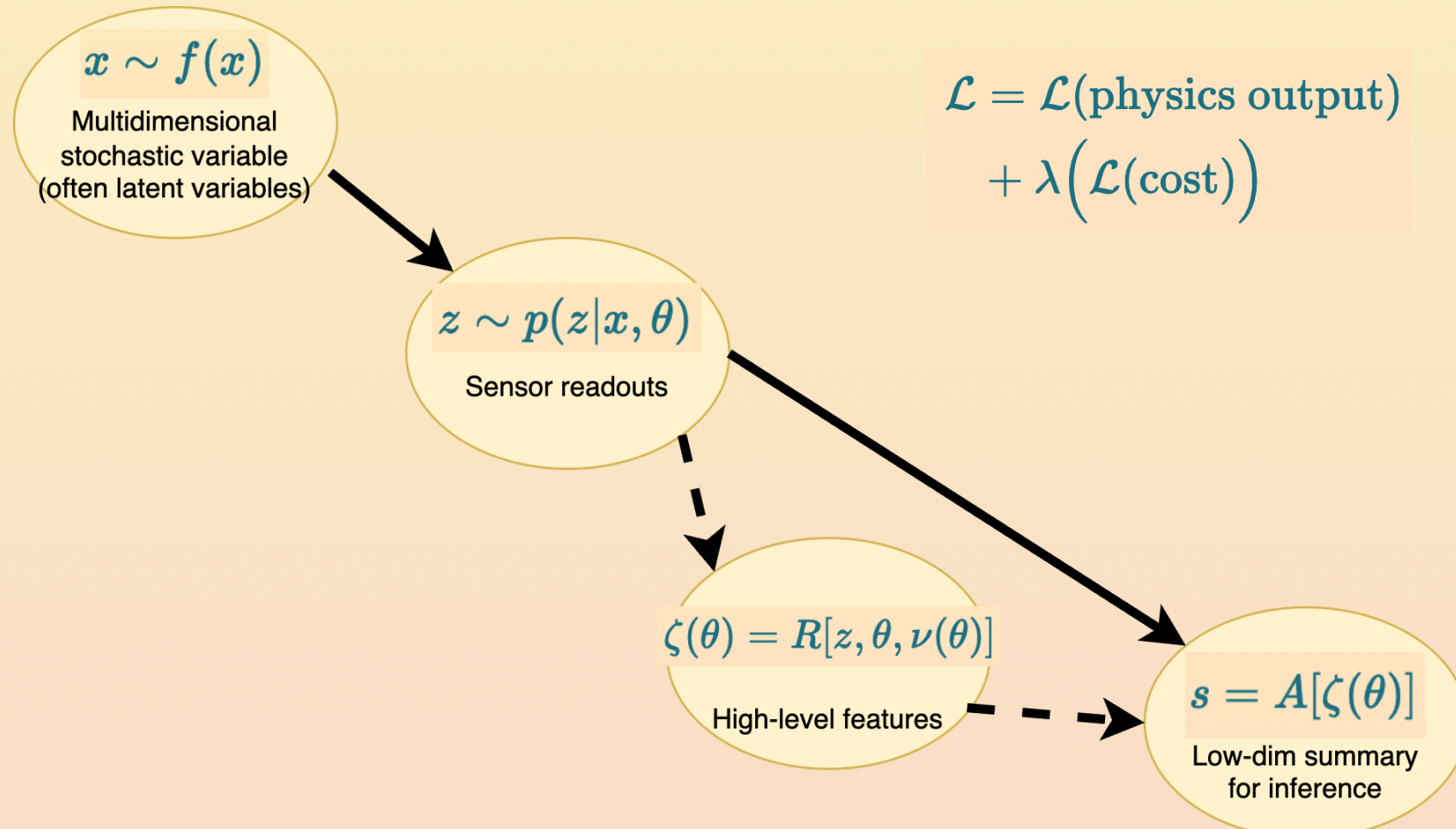
Important note: this won't be sufficient to take us to "true" AI. Other concepts will be needed for that, such as what I used to call predictive learning and now decided to call Imputative Learning. More on this later...

👍 1.8K

186 Comments 464 Shares

Measurement-aware detector opt.!

- Joint optimization of design parameters w.r.t. inference made with data
- MODE White Paper, [10.1016/j.revip.2023.100085 \(2203.13818\)](https://arxiv.org/abs/2203.13818), 117-page document, physicists + computer scientists



Feasibility within constraints

Depends on z and nuisances

Cost of the layout with parameters θ

Closed form

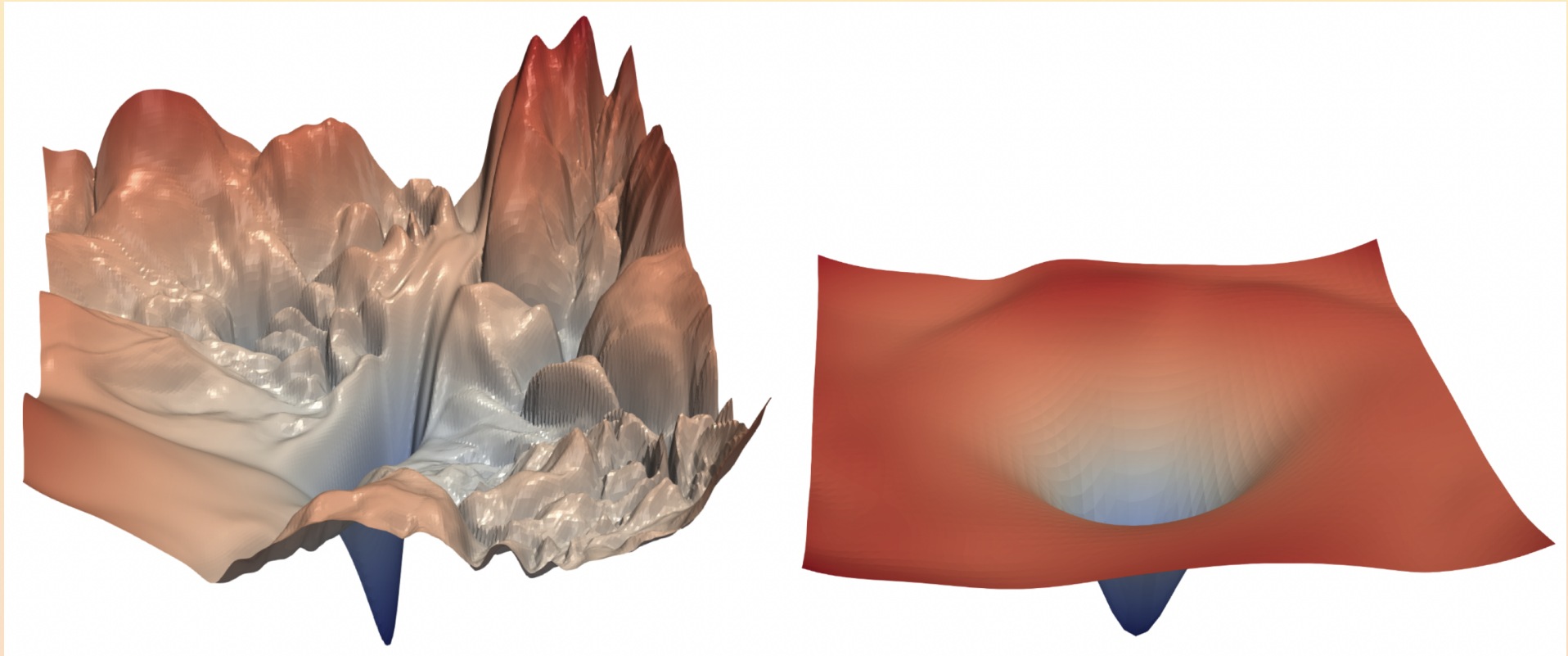
$$\hat{\theta} = \arg \min_{\theta} \int L[A(\zeta), c(\theta)] p(z|x, \theta) f(x) dx dz ,$$

Weight desirable goals while obeying cost constraints

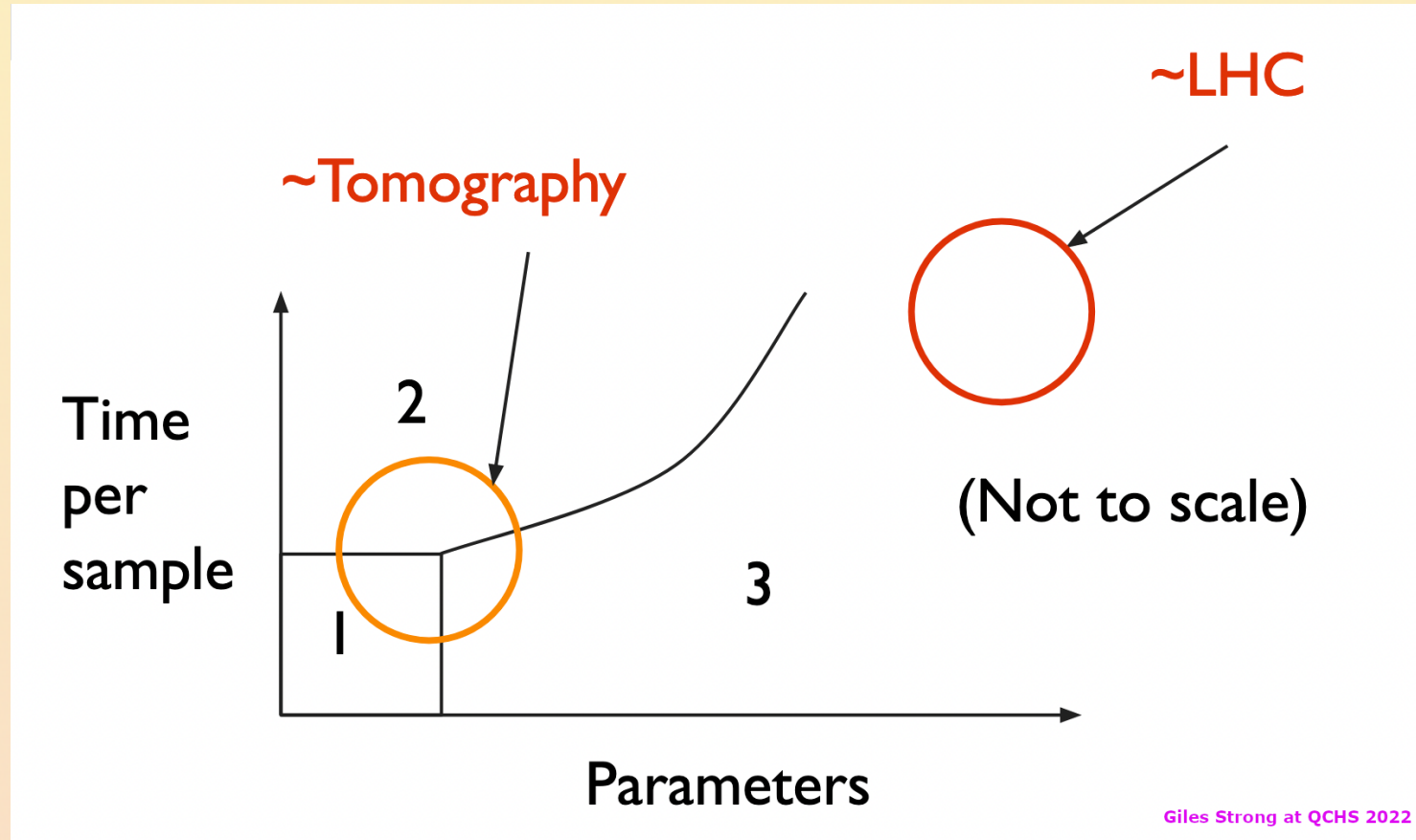
- Costs can be monetary but also any case-specific technical constraint
 - Local, specific to the technology used (e.g. active components material)
 - Global, describing overall detector conception (e.g. number, size, position of detector modules)
- Fixed costs can be added separately to the loss function

Assist the physicist with a landscape of solutions

- Results are as good as your parameterization: **cannot parameterize everything!**
- "**The optimal solution**" is unrealistic: provide **feasible solutions near optimality**
- The physicist will fine tune



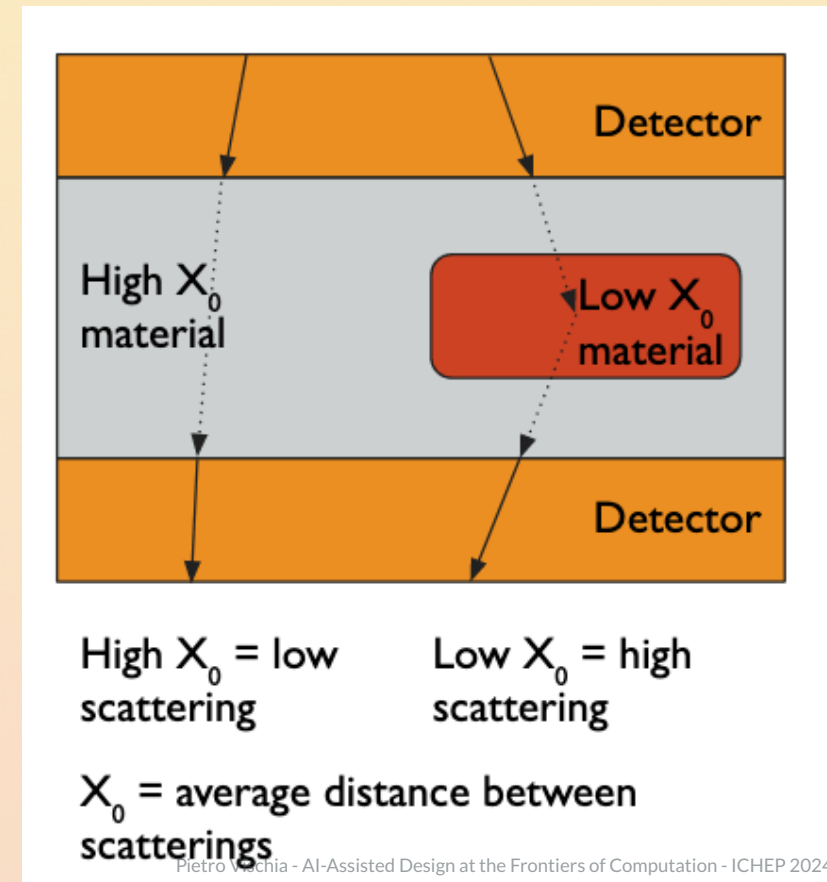
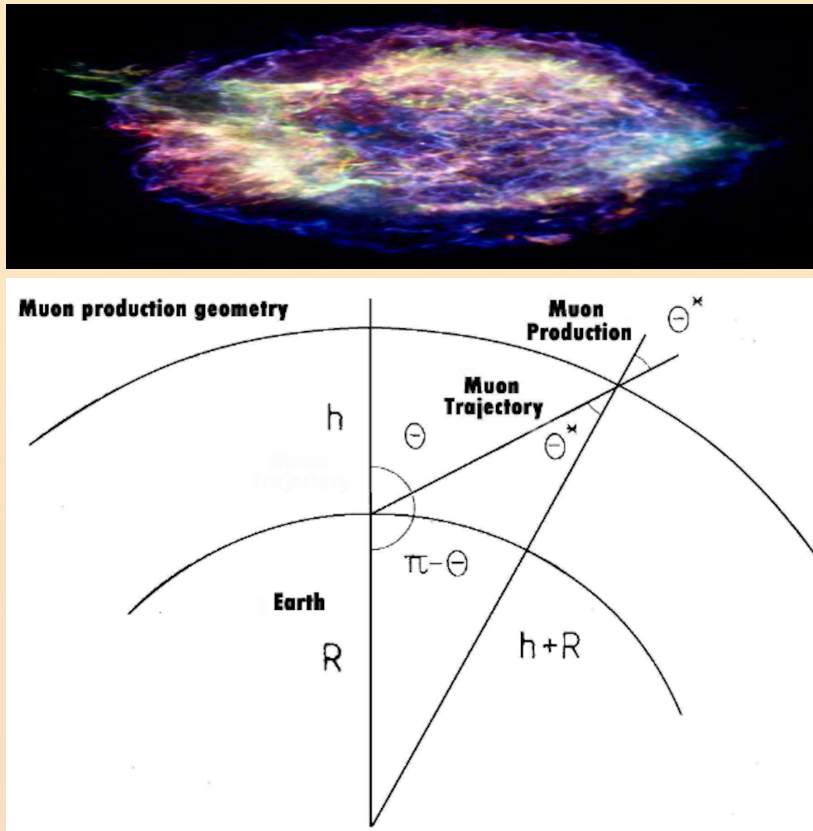
Method of choice depends on scale



1. Grid/random search
2. Bayesian opt, simulated annealing, genetic algos, ...
3. Gradient-based optimization (Newton, BFGS, gradient descent, ...)

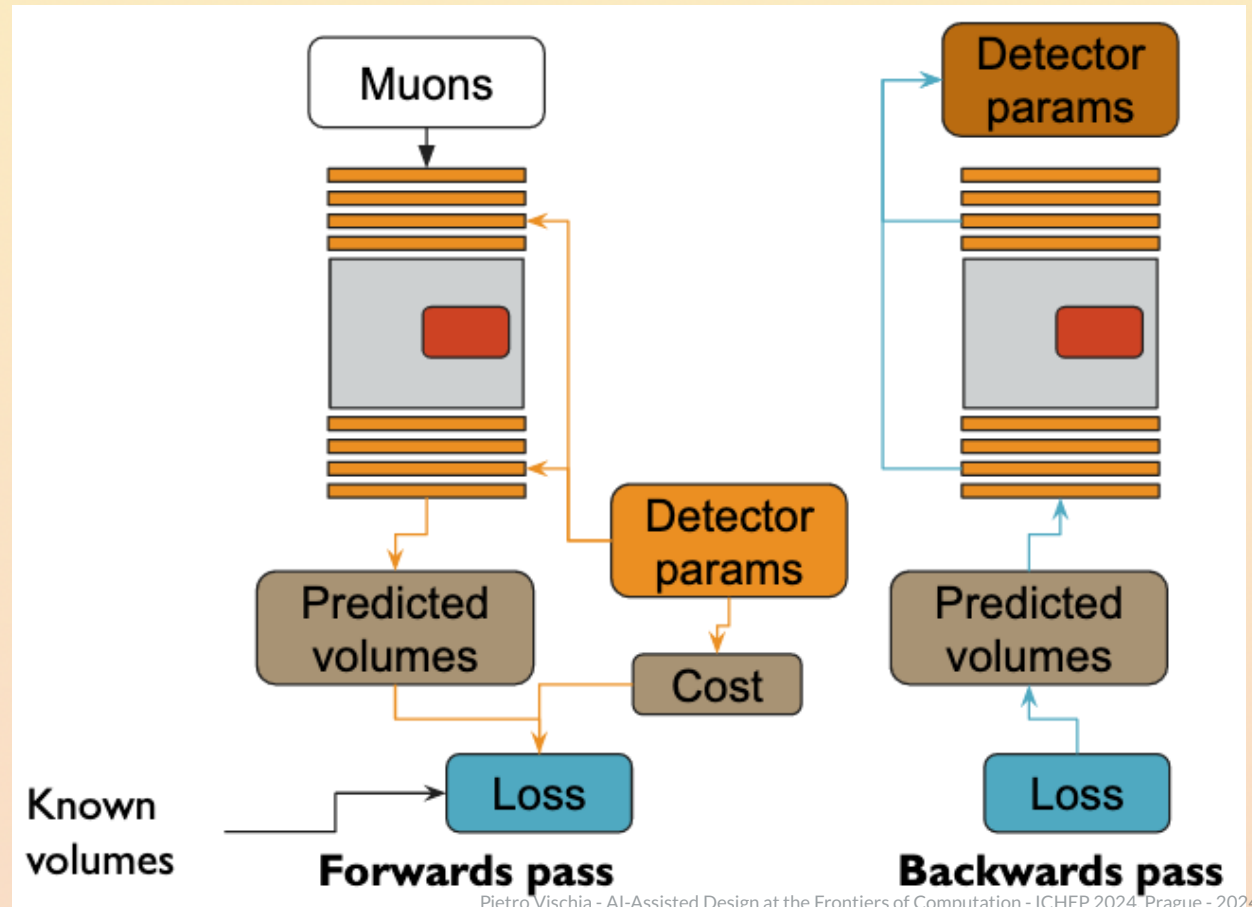
Muon tomography

- Muons from high-energy primary cosmic rays that impact with the atmosphere
- Infer properties (e.g. 3D map of elemental composition X_0) of unknown volume: stochasticity!
- Tomography by **absorption** (measure missing flux, e.g. pyramids, volcanoes) or **scattering** (measure deflection, e.g. containers, furnaces, statues)



TomOpt

- Differential optimization of muon-tomography detectors
 - [10.1088/2632-2153/ad52e7](https://arxiv.org/abs/10.1088/2632-2153/ad52e7): presented at NeurIPS MLPS Workshop, published two weeks ago in *Machine Learning: Science and Technology*
 - Modular design in python, autodiff via PyTorch
- Inference chain as differentiable pipeline
 - Can compute $p(\Delta output | \Delta detector\ parameters)$
- Task as loss function
 - Including target (e.g. prediction uncertainty), costs, constraints
- Backpropagate and optimize as usual
 - Gradient descent



Optimize a parametric design under constraints

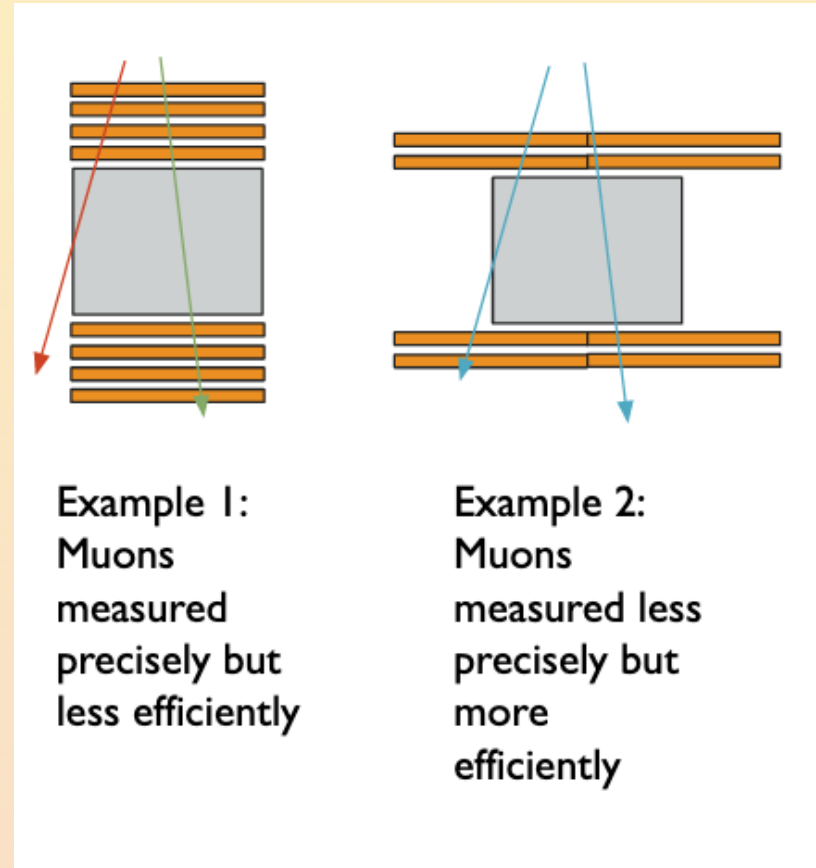
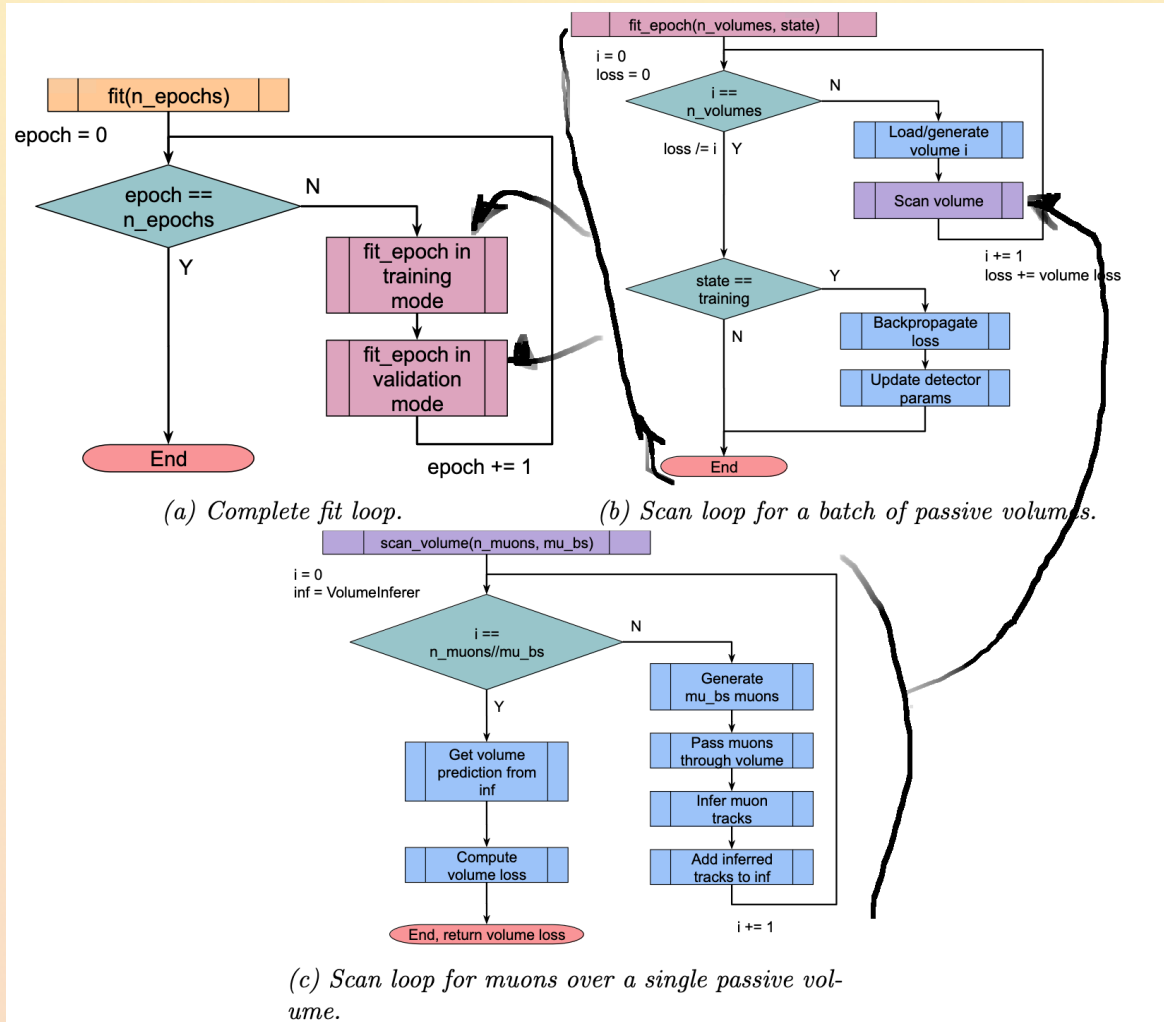
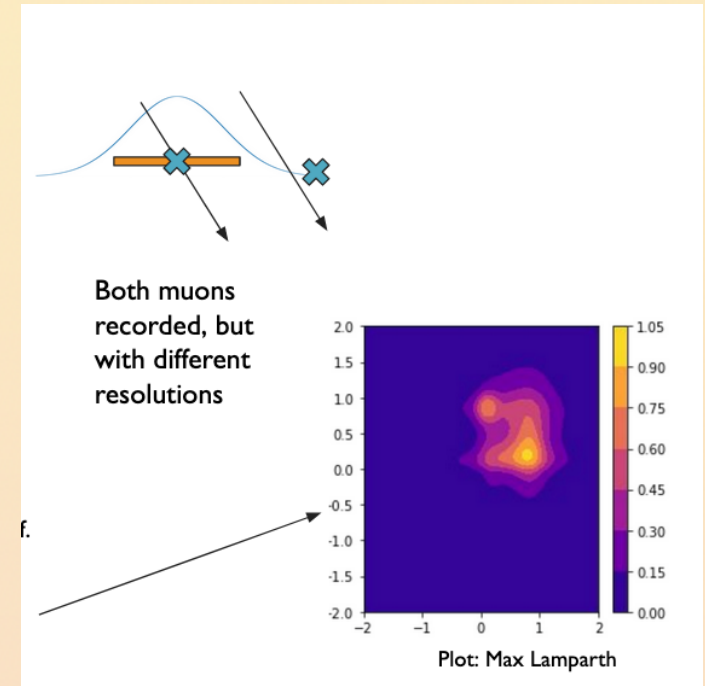
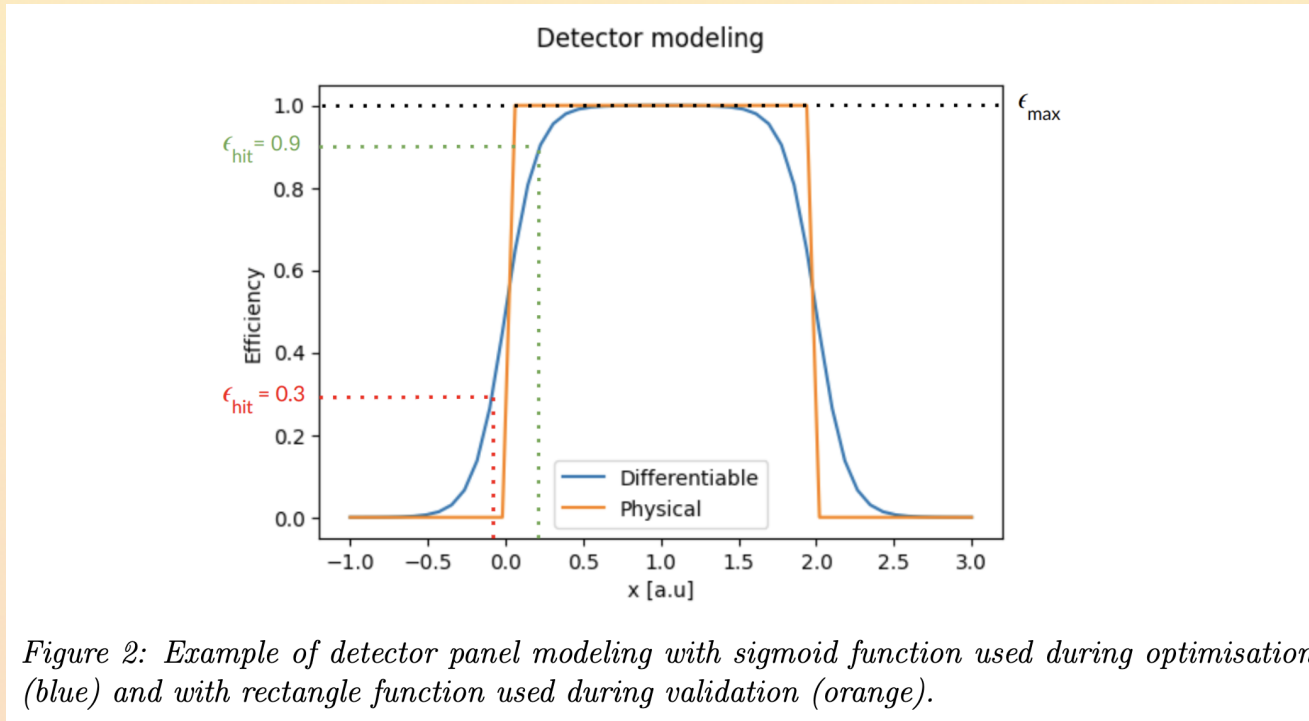


Figure 6: Breakdown of the fitting procedure of detectors in TOMOPT

Make things differentiable

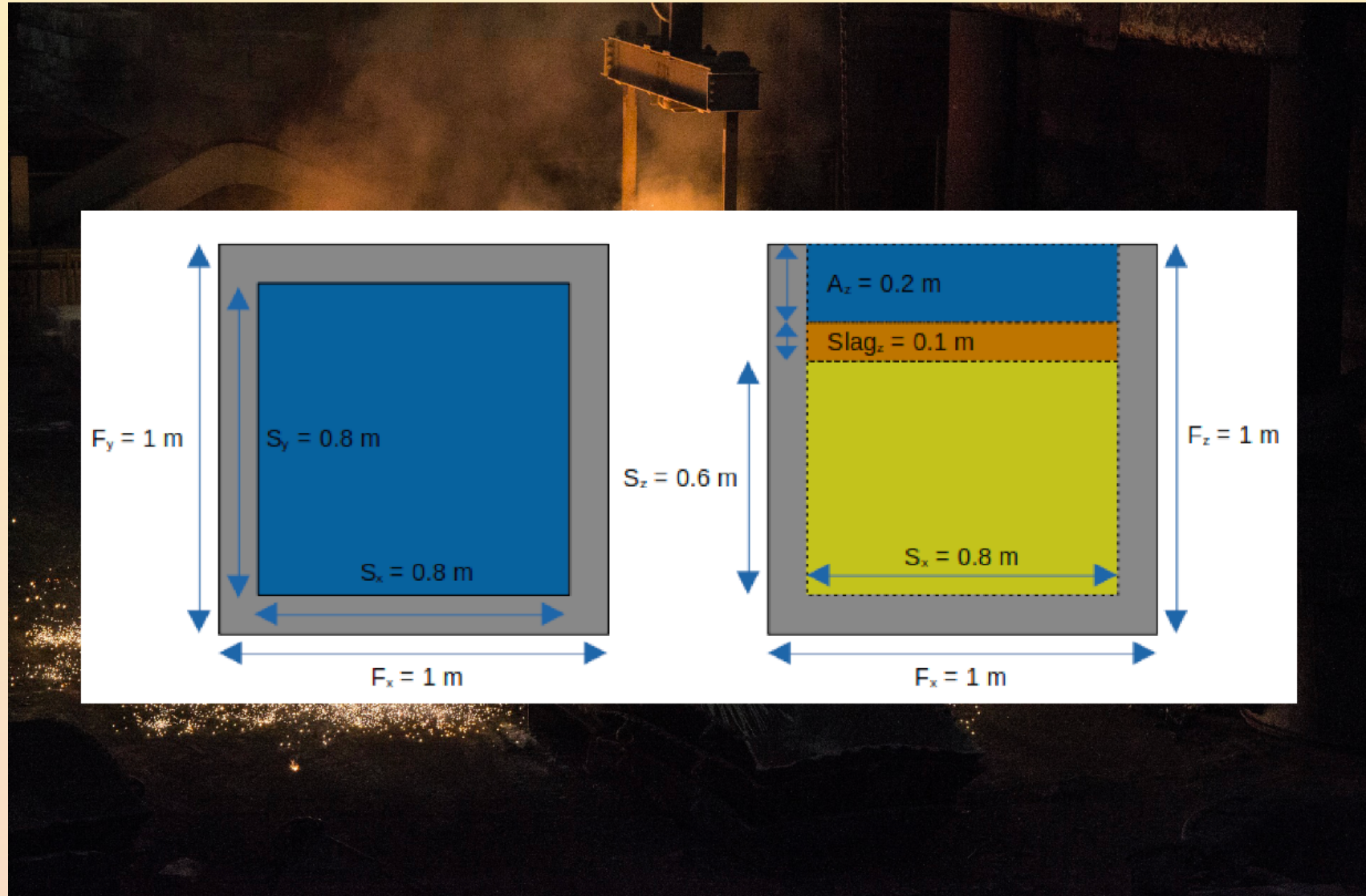
- Panels made differentiable only during training
- Associate to a muon hit a distribution based on resolution and efficiency



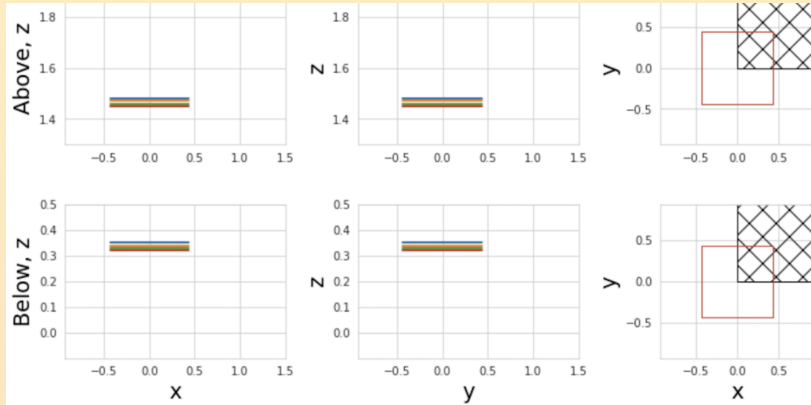
Heavy-Metal Benchmark



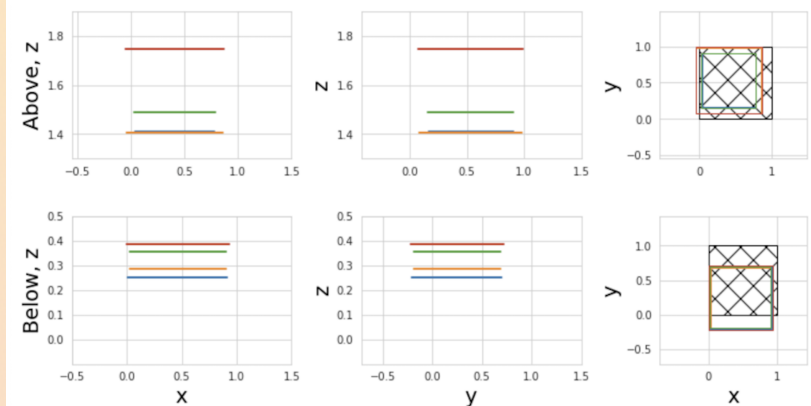
Heavy-Metal Benchmark



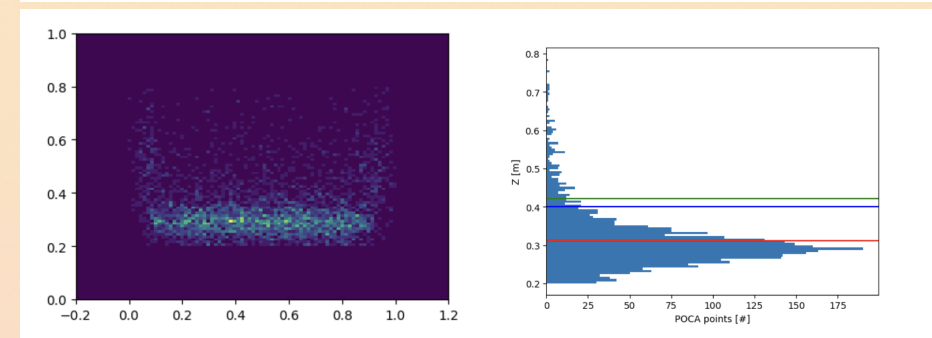
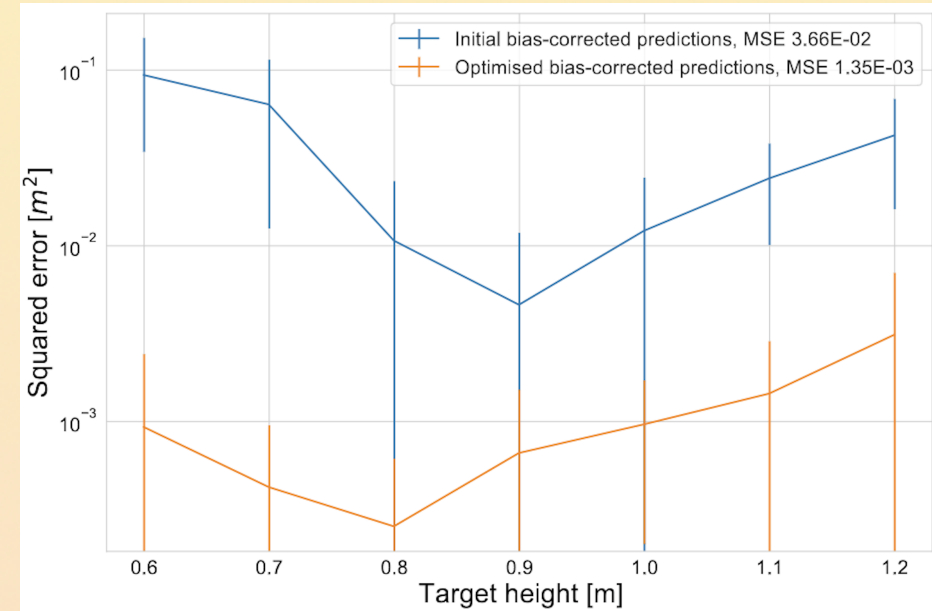
Optimized design is more performant



(a) Initial detector configuration.



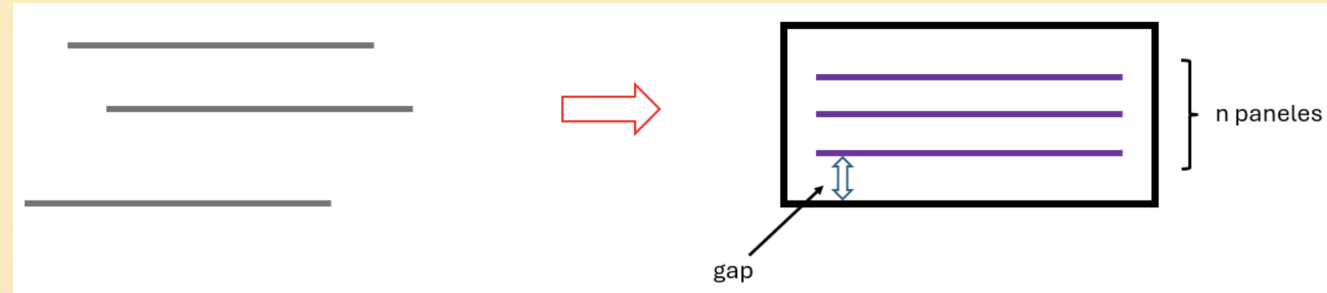
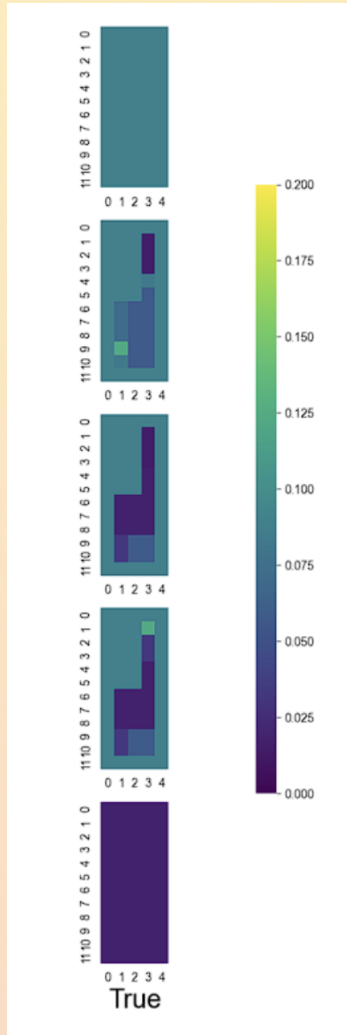
(b) Detector configuration after stage one optimization process.



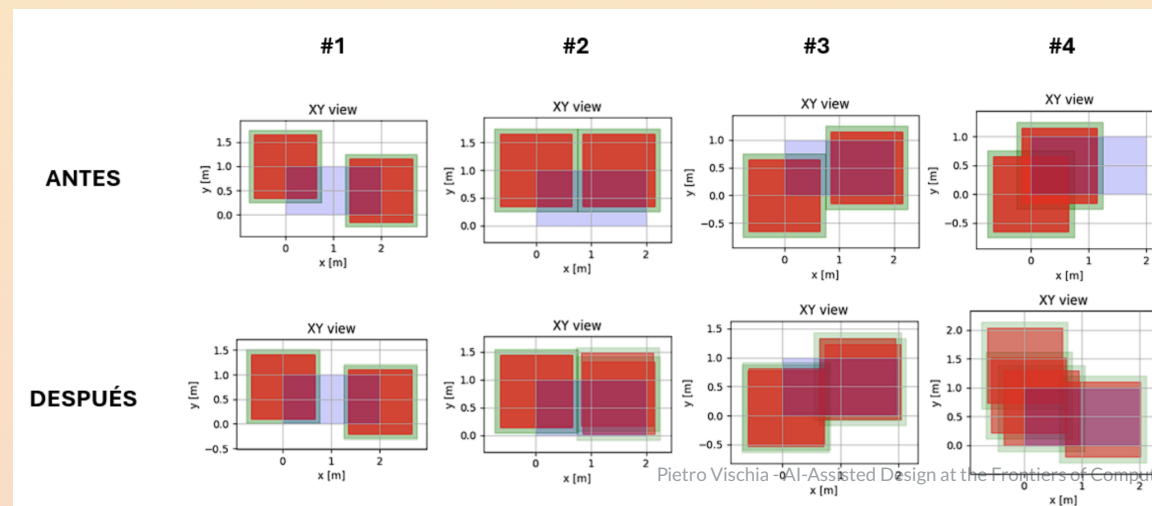
(Blue: true steel level. Red: prediction. Green: bias-corrected prediction)

Extension: hodoscopes

- Setup from European plan for border control: hodoscope structure already decided, only placement can be changed

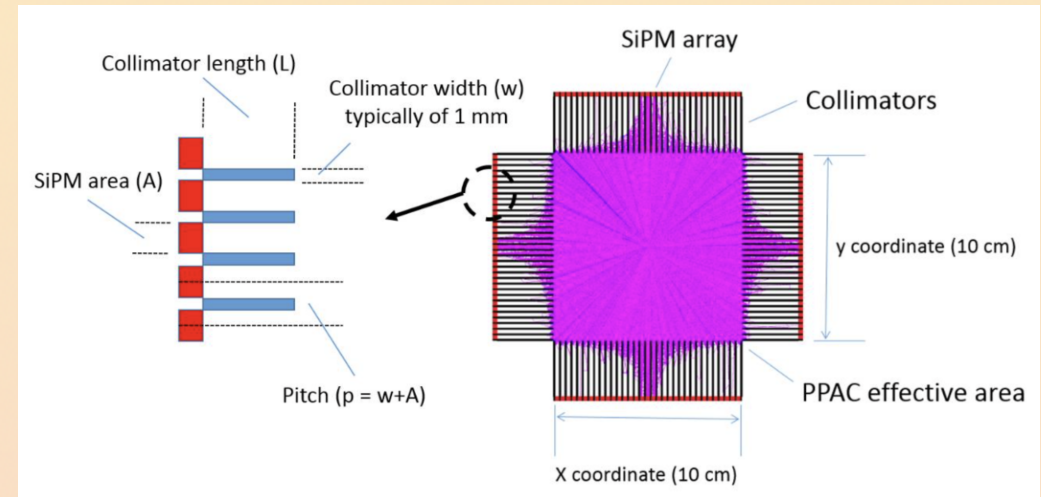
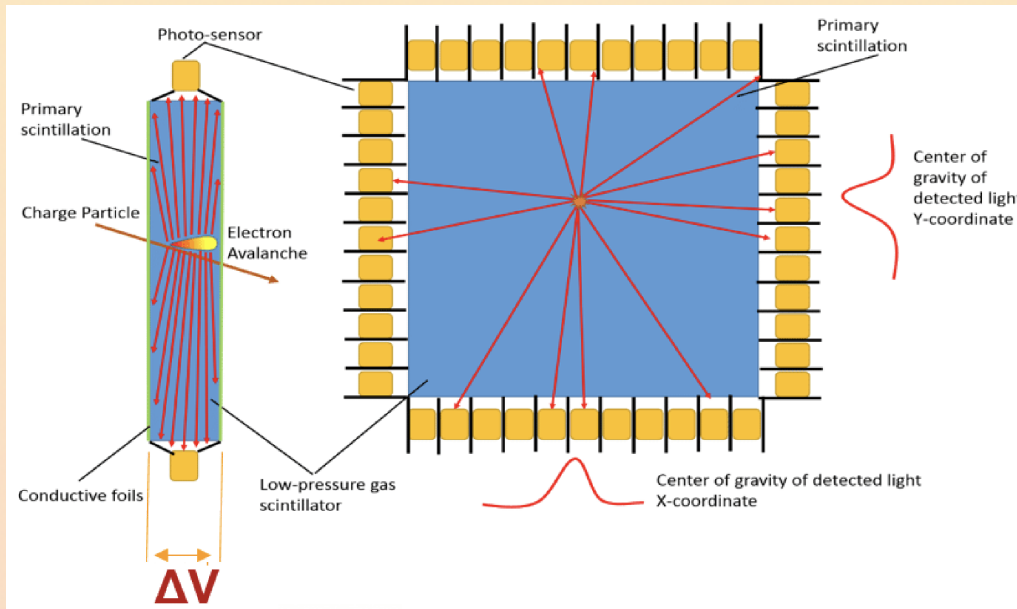


- Scan a lorry: significant code restructuring to account for hodoscope structure
- Accepted by the MARESEC conference for paper publication
 - [Zaher, Lagrange, Álvarez Lueje et al. \(PV\), 2024](#) (BSc thesis of Samuel Álvarez Lueje)



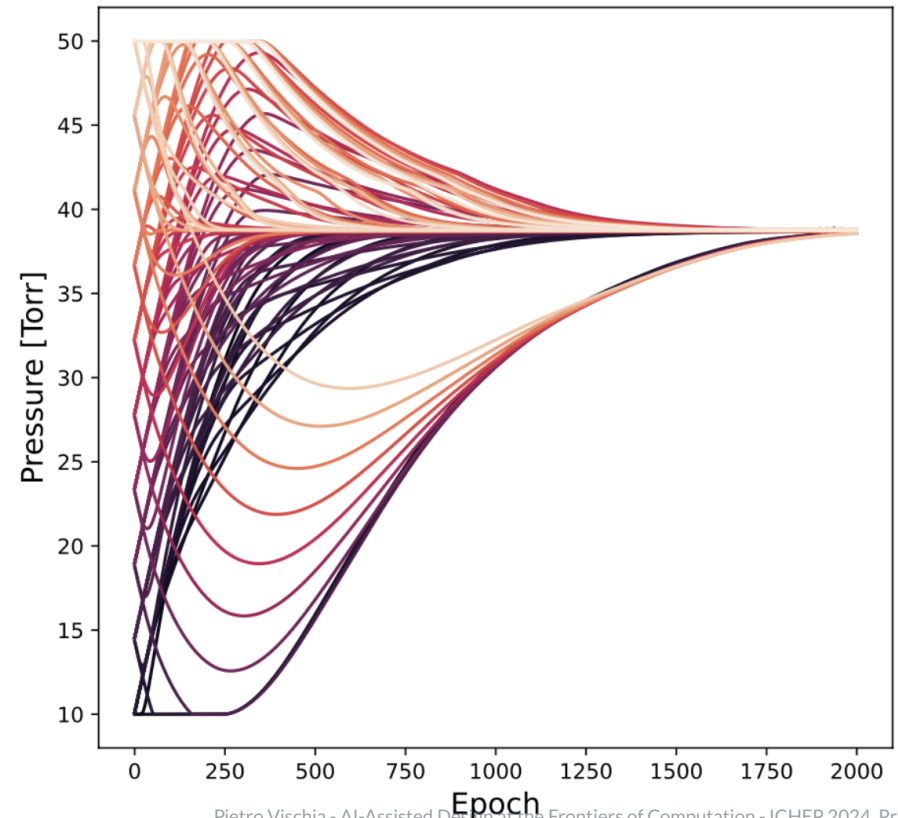
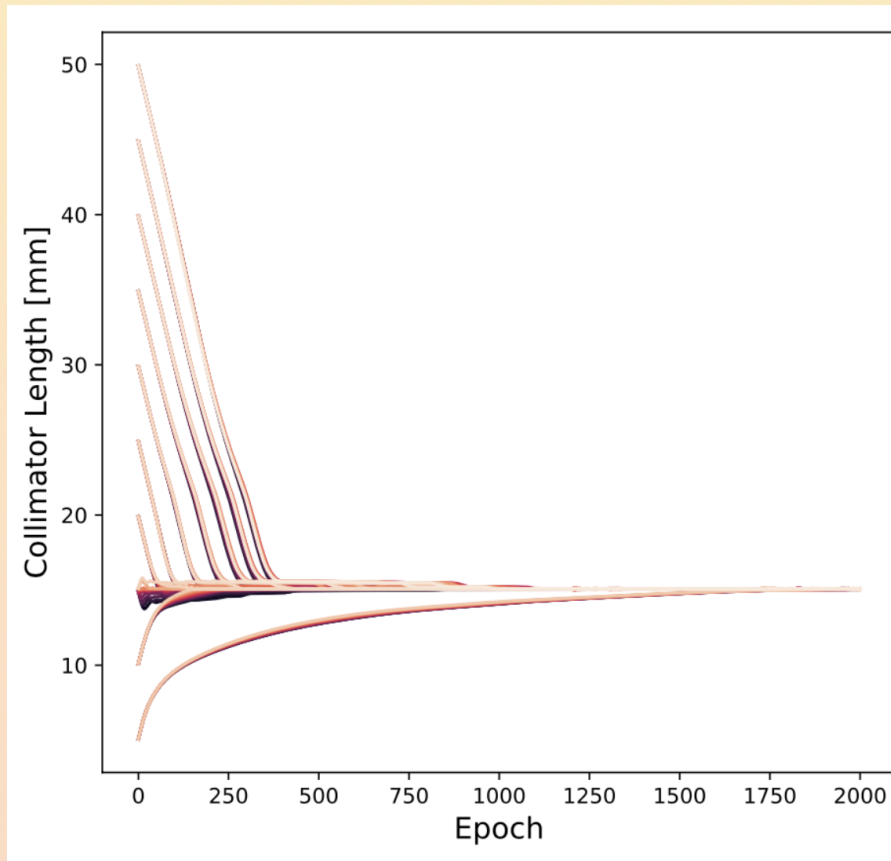
Neutron Tomography

- GEANT4 model of a $10 \times 10\text{cm}^2$ O-PPAC (Parallel-Plate Avalanche Counter with Optical Readout) from *Neutron Insights*
 - Parallel electrodes with 3mm gap filled with low-pressure scintillating gas mixture (CF₄) with high electroluminescent light yield
 - Readout via array of small silicon photomultipliers SiPMs
- Parametric neural network surrogate of the GEANT4 simulation
 - p : higher pressure \rightarrow higher electroluminescence yield (up to a threshold), but larger voltage (energy expenditure)
 - L : collimator length: tradeoff between accurate light localization (high L) and higher photon statistics (low L)



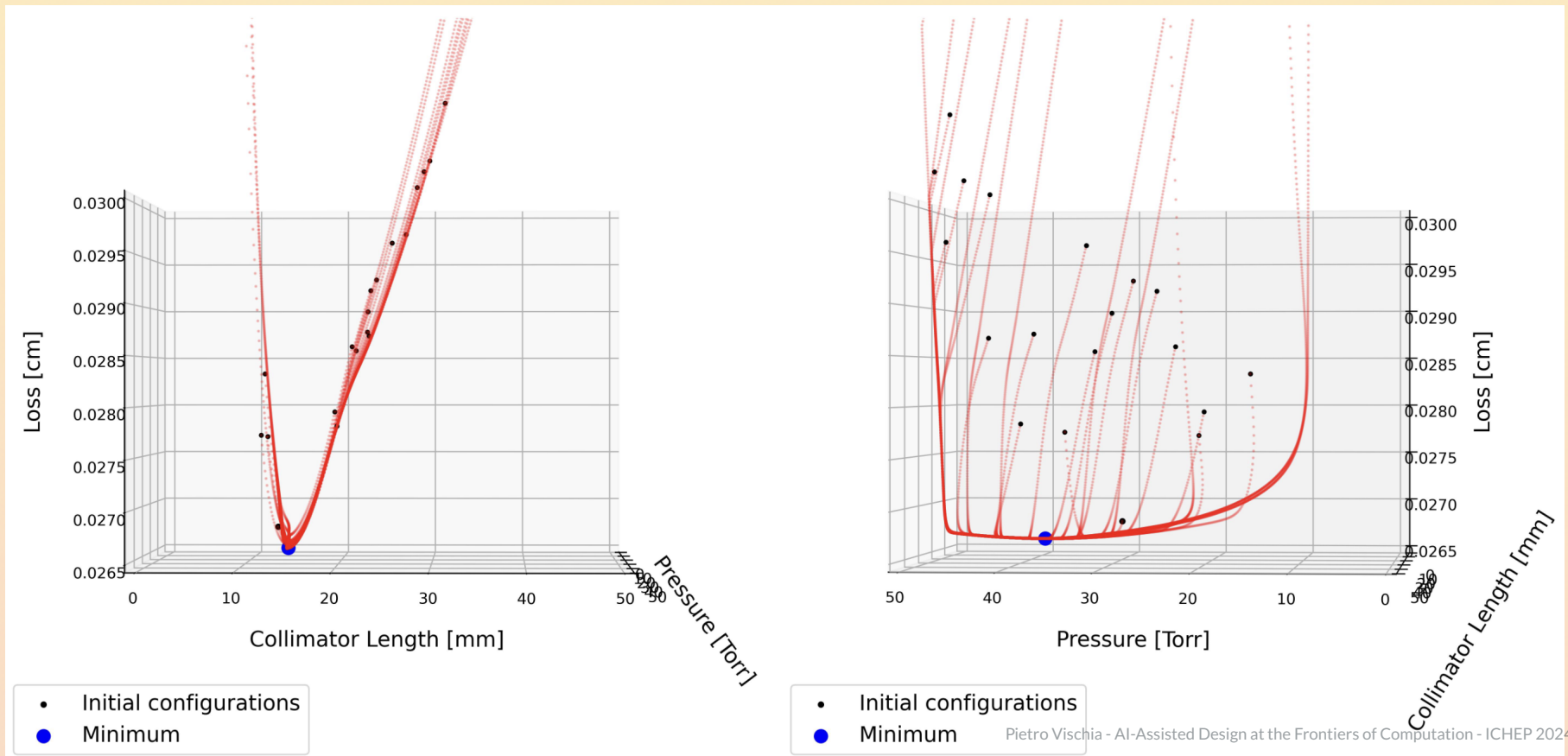
Neutron Tomography: optimization

- Results for L give the same result as traditional studies from [10.1088/1748-0221/13/10/P10006](https://doi.org/10.1088/1748-0221/13/10/P10006)
- Remarkably stable **regardless of initial configuration**
- [MSc thesis of María Pereira Martínez](#)
 - Paper in preparation (w/ M.P.M., Xabier Cid Vidal)



Neutron Tomography: optimization

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Thrive in asymmetries or lack thereof

2006: genetic algorithms



2024: SWGO tanks placement optimization

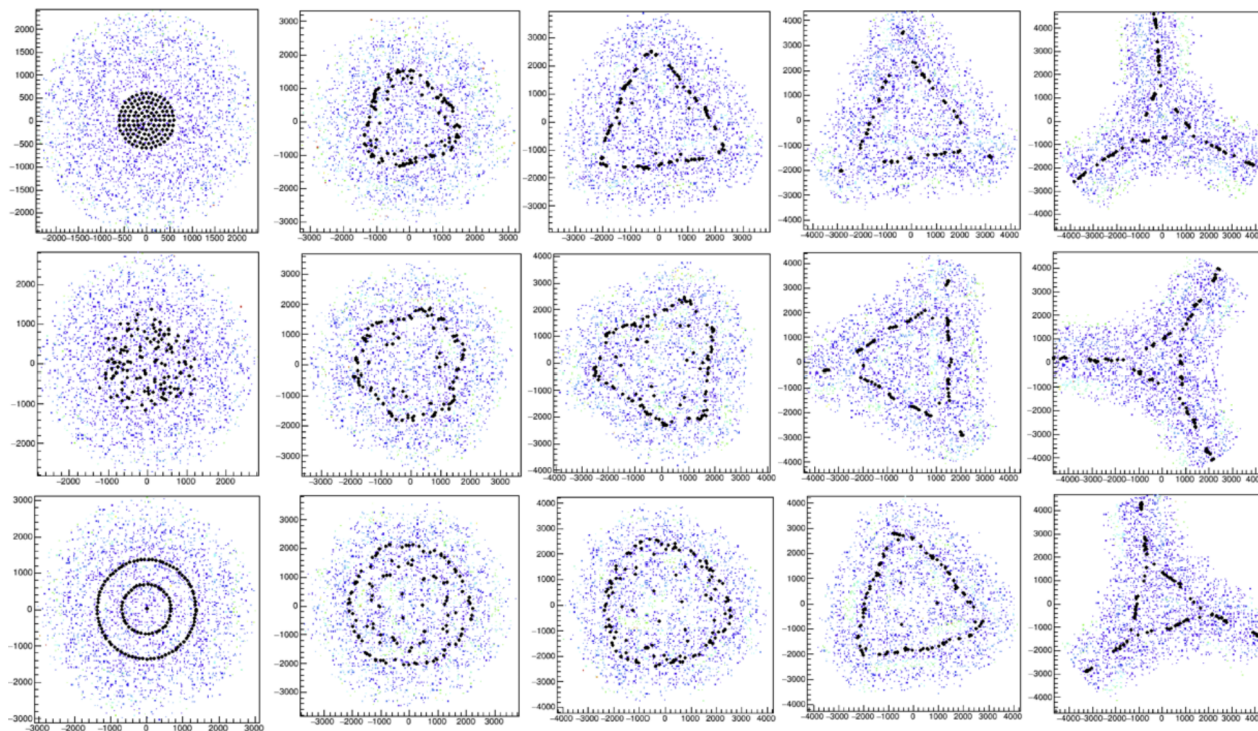
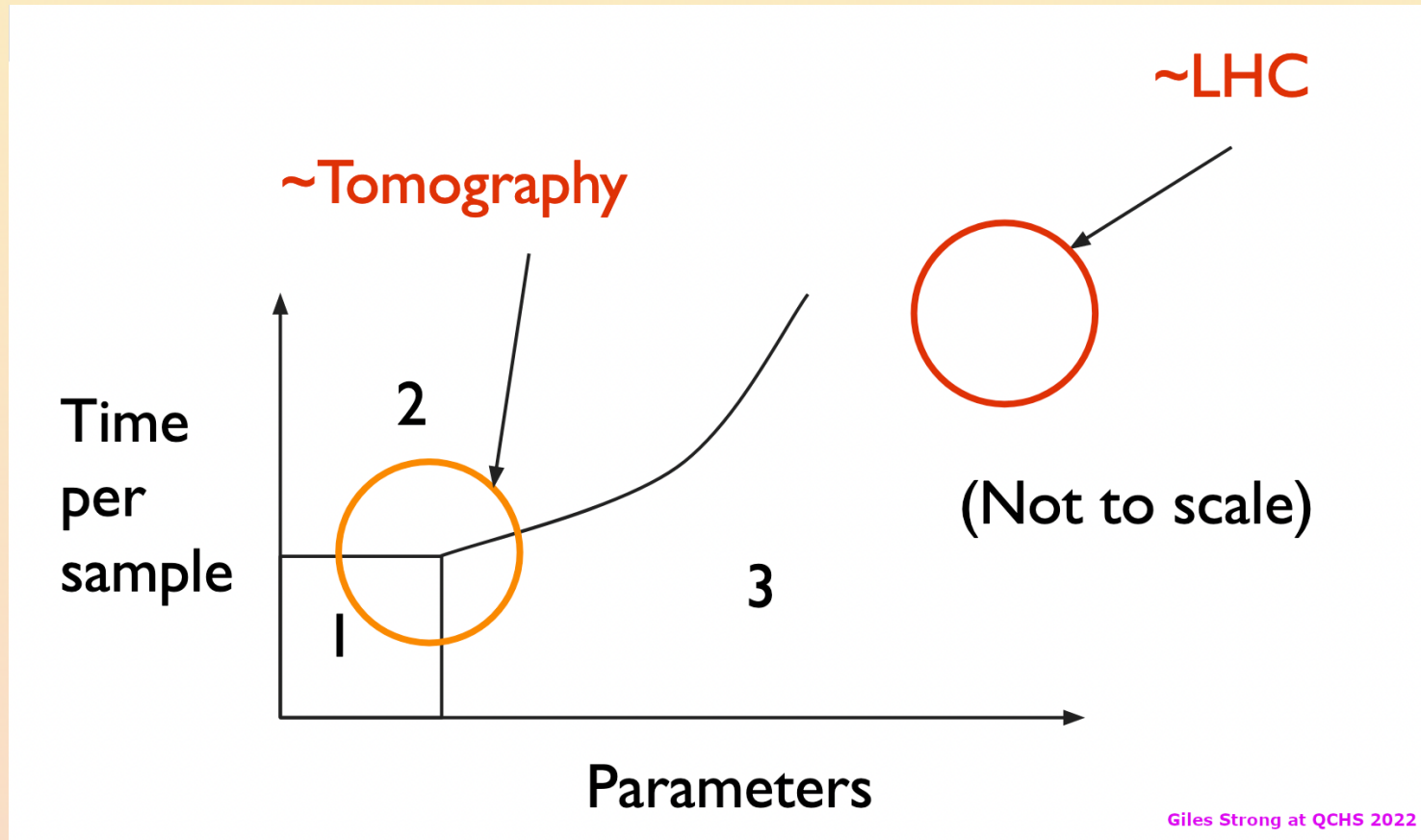


Figure 14: Convergence of three initial layouts (top to bottom: packed ball, wide random ball, two annuli) during a 500-epochs training. From left to right, the configurations of 126 units (129 in the bottom one) are shown at epoch 1,50,150,300, 500. See the text for more detail.

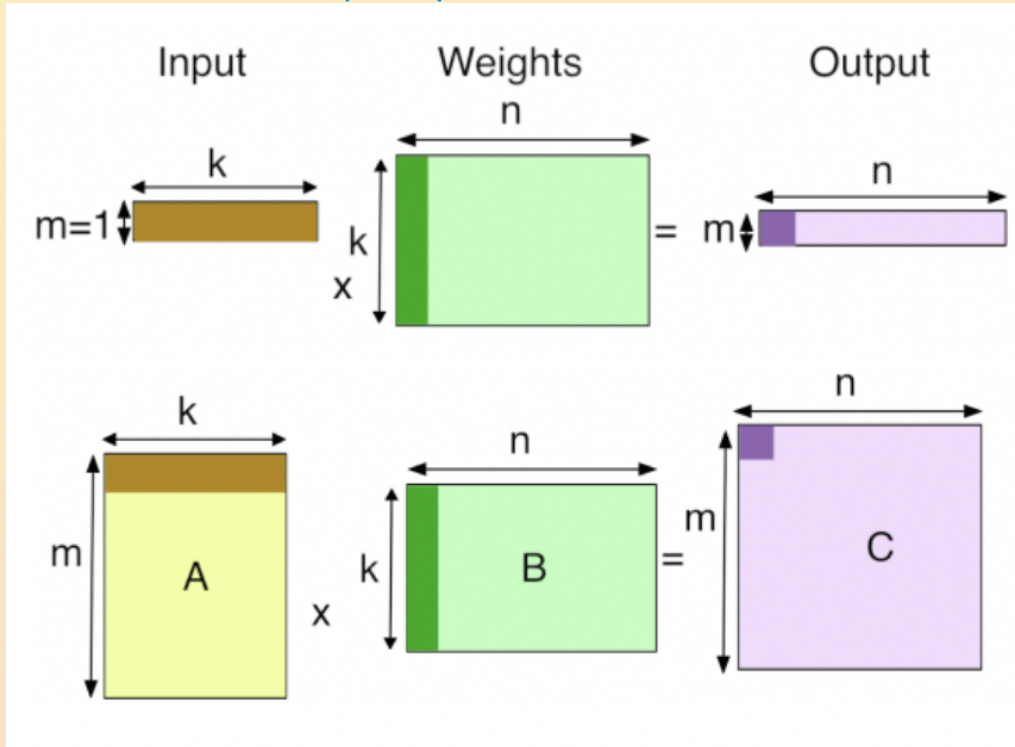
Experimental design: present and future

- Gradient descent applied to experiment design works!!!
 - Discreteness and stochasticity mostly solvable or avoidable
- Can we make it scale?

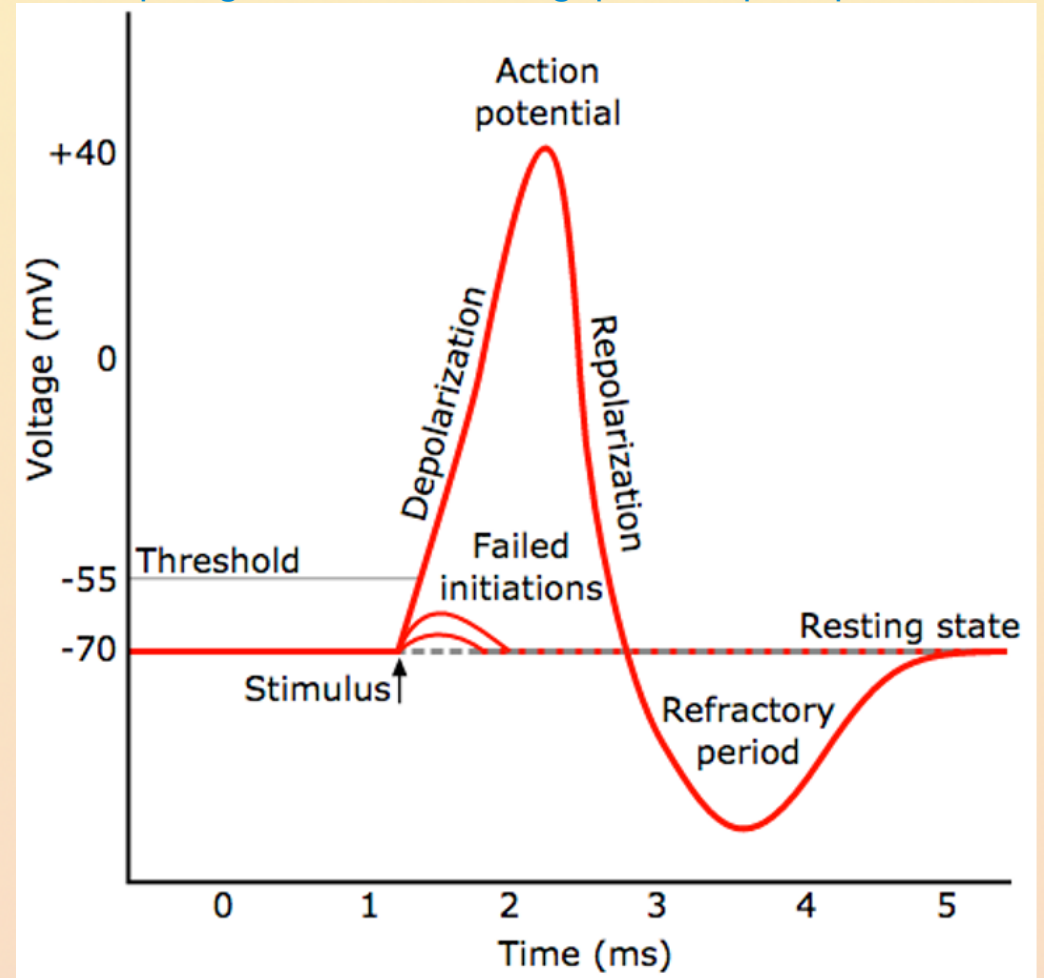


Paradigm shift

From perceptrons and matrices...



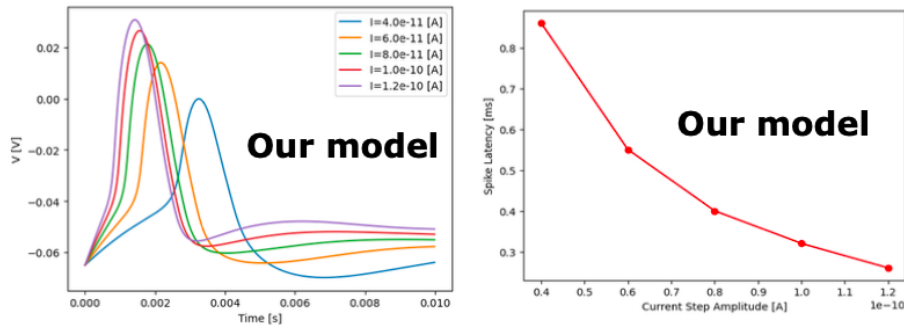
to spiking neurons modulating spatiotemporal patterns



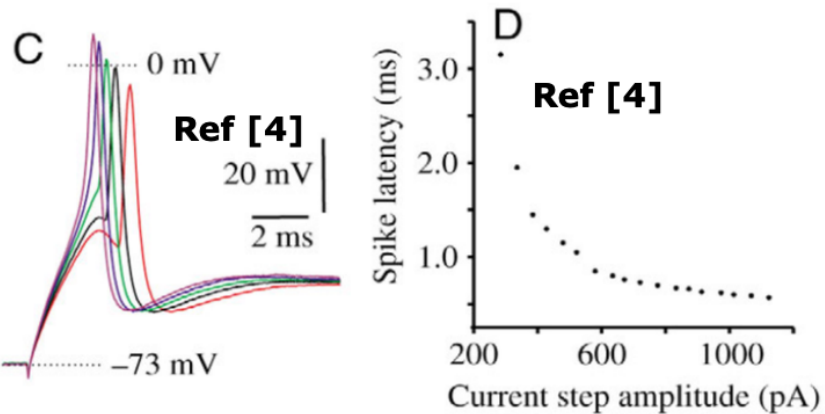
Realistic models for biological neurons

- Spherical neuron with four channels (different thresholds and time constants) for *Gymnotus Omarorum*
 - Vischia, Caputi 2023: computational model compared with data from "[4]" (J Exp Biol (2006) 209 (6): 1122–1134.)

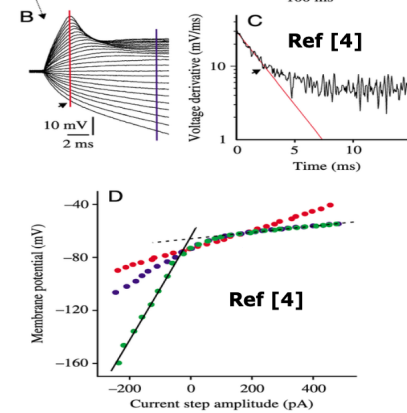
- The amplitude of the stimulus step drives the spike latency



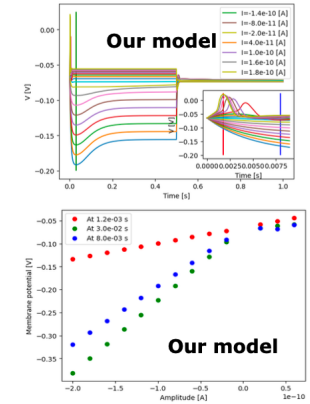
- Observations exhibit the same behaviour
- Further turning needed for the spike shape



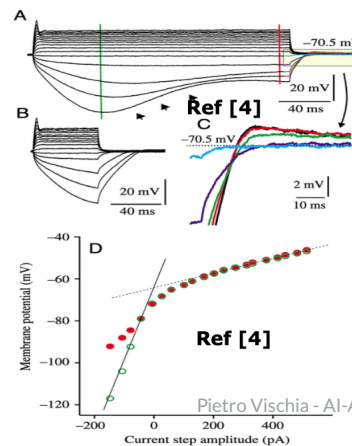
- Early subthreshold responses



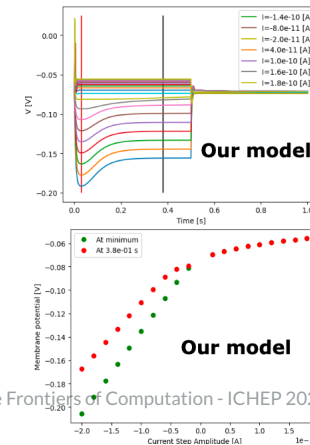
- Before hump (red), linear V-I relation
- After hump, for depolarizing steps V-I relation is nonlinear
The activated conductance does not inactivate at later times



- Late subthreshold responses



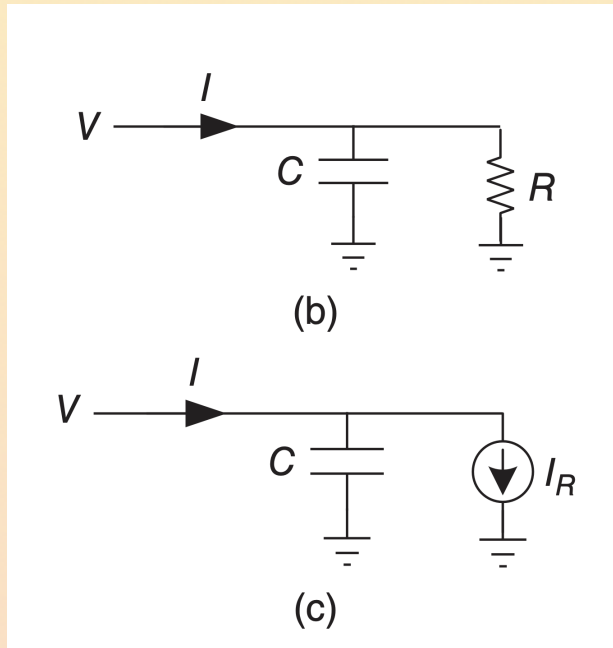
- At peak hyperpolarization, limiting slope is maximal
- At end of the step, depolarization curves decay much faster



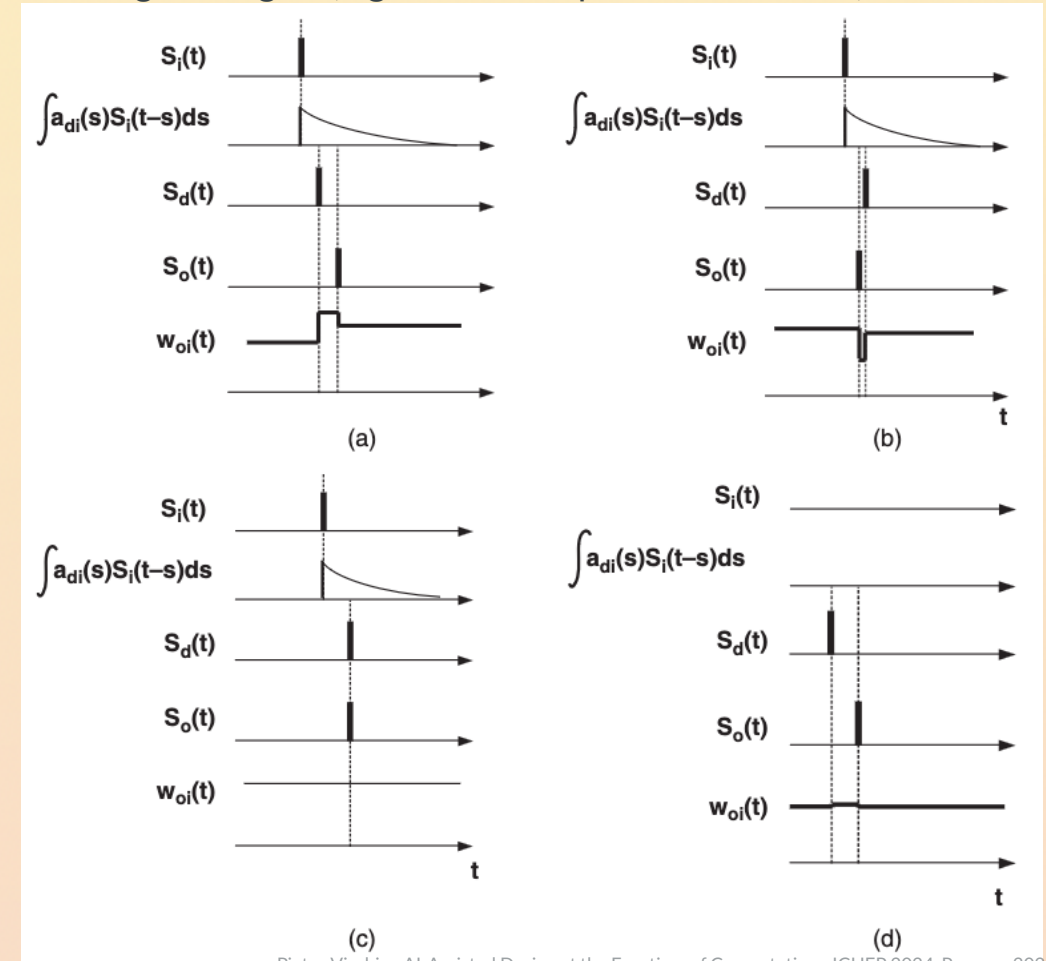
Spiking networks

- Neuronal model vastly simplified: the (Leaky) Integrate-and-fire Model

$$C \frac{dV(t)}{dt} = I - I_L$$



Training strategies (e.g. [Remote Supervised Method](#))



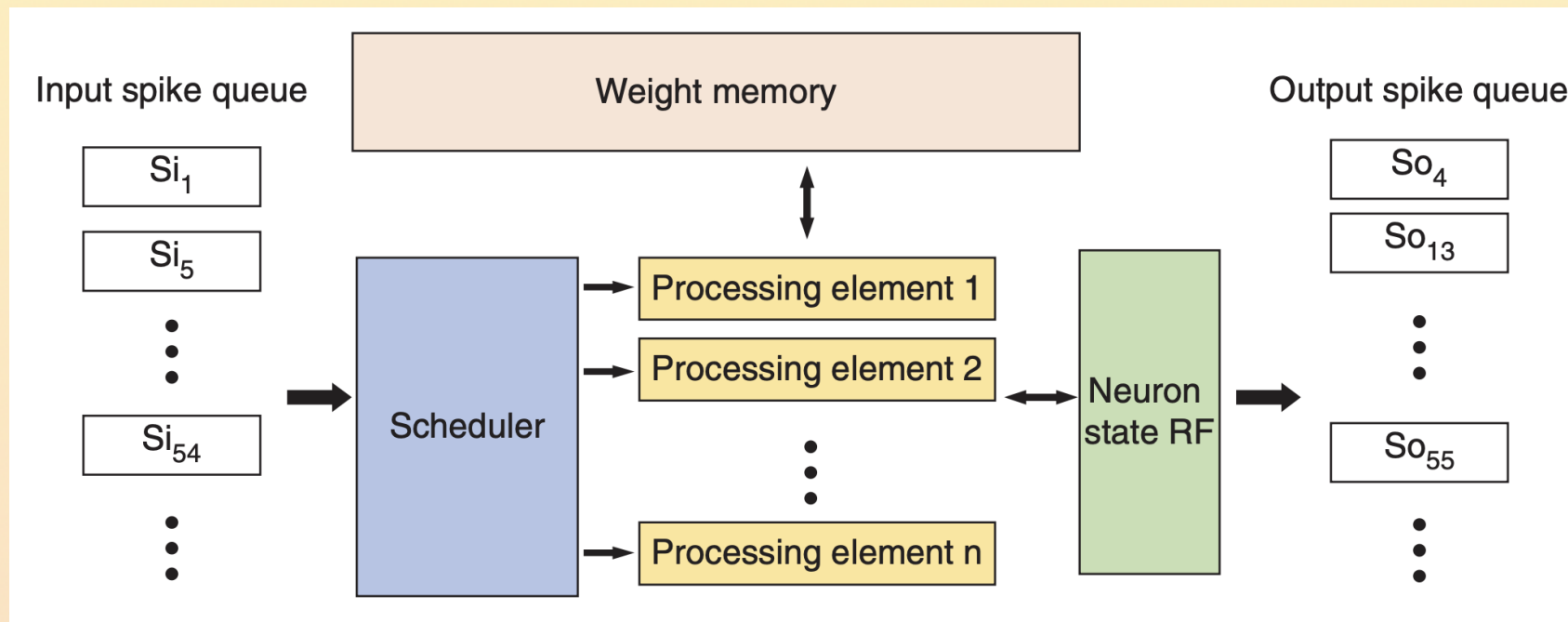
Event-driven computation

- Event-driven computations
 - "when a spike occurs, compute something": realtime operations by reducing bus width ($N_{axons} \rightarrow \log_2 N_{axons}$) in CMOS or memristors
 - Work in progress on various applications
 - Q-Pix (see talk by [Shion Kubota](#)) uses same natural representation: maybe synergies?



Energy-efficient architectures

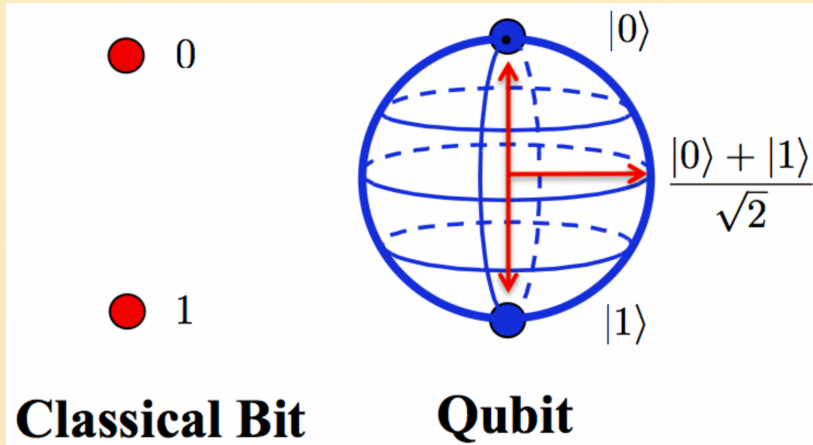
Sparser inputs → less time and energy



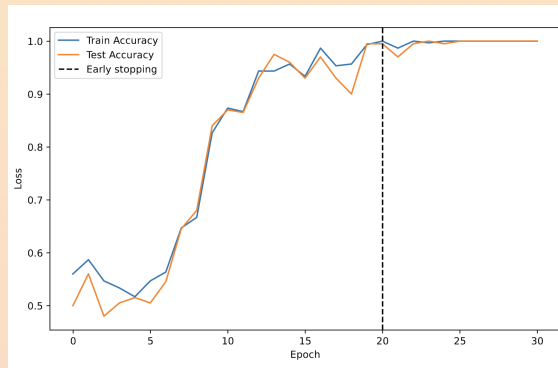
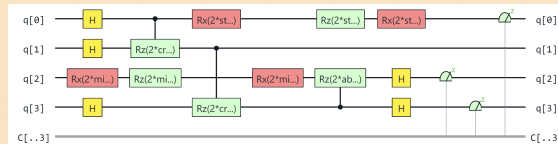
	Brain	Spikey	SpiNNaker	R2600X	Intel mobile	RTX2070
Housekeeping	4.75E-11	1.37E-06	1.66E-04	4.49E-04	1.23E-04	9.76E-07
Resting potential	5.77E-11	3.83E-08	8.99E-05	4.77E-05	4.25E-05	3.63E-06
Action potential	1.96E-11	4.39E-10	1.04E-08	3.04E-08	4.46E-09	4.71E-09
Transmission	8.17E-15	1.08E-11	9.59E-09	5.82E-08	2.14E-08	3.40E-09
Single neuron	2.49E-10	1.49E-06	3.33E-04	9.62E-04	3.37E-04	3.18E-05
Full brain	2.15E+01	1.29E+05	2.87E+07	8.29E+07	2.90E+07	2.74E+06

Values for the simulation of 1s of model time are reported in Joule. The single neuron and full brain estimates assume a fan-out of 2,000 synapses and a spike rate of 4Hz. R2600X: AMD Ryzen 2600X. Intel mobile: Intel Core i7-4710MQ. RTX2070: NVIDIA RTX 2070. Both CPUs are measured using a PeakTech power meter. The lowest values from simulators/emulators are highlighted in bold.

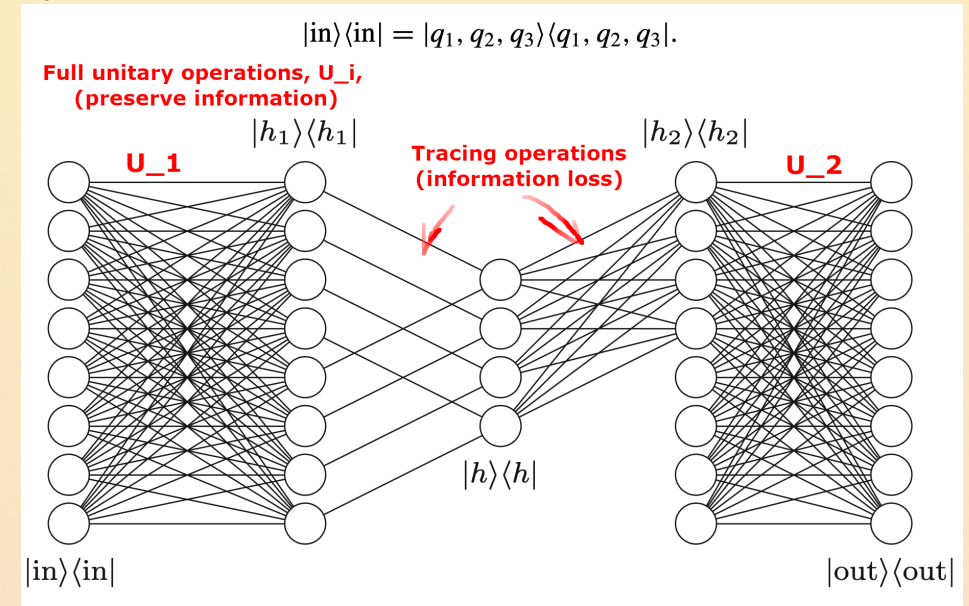
Differentiable quantum optimization



- Quantum representation can have advantages
 - Lower dimensional, and achieving high efficiency with small datasets
 - BSc thesis of Manuel Uría García (paper in preparation M.U.G. and José M. Uría (UriaXait SL))



- Natural representation of neural networks by qubit operations



- Gradient descent exploits intrinsic **analytic differentiability** of quantum circuits

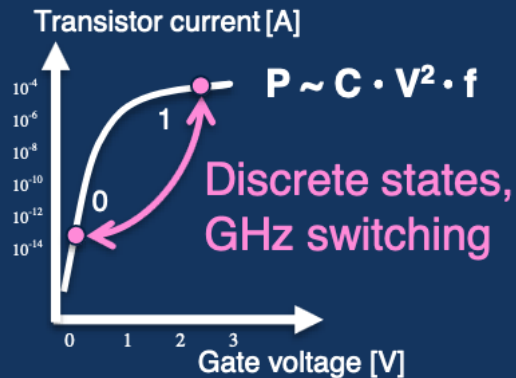
$$\begin{aligned}
 \partial_\mu \langle \psi(x, \theta) | \sigma_z | \psi(x, \theta) \rangle &= \langle 0 | \dots \partial_\mu e^{-i\mu\sigma} \dots \sigma_z \dots e^{i\mu\sigma} \dots | 0 \rangle \\
 &\quad + \langle 0 | \dots e^{-i\mu\sigma} \dots \sigma_z \dots \partial_\mu e^{i\mu\sigma} \dots | 0 \rangle \\
 &= \langle 0 | \dots (-i\sigma) e^{-i\mu\sigma} \dots \sigma_z \dots e^{i\mu\sigma} \dots | 0 \rangle \\
 &\quad + \langle 0 | \dots e^{-i\mu\sigma} \dots \sigma_z \dots (i\sigma) e^{i\mu\sigma} \dots | 0 \rangle \\
 &= \langle 0 | \dots (1 - i\sigma) e^{-i\mu\sigma} \dots \sigma_z \dots (1 + i\sigma) e^{i\mu\sigma} \dots | 0 \rangle \\
 &\quad + \langle 0 | \dots (1 + i\sigma) e^{-i\mu\sigma} \dots \sigma_z \dots (1 - i\sigma) e^{i\mu\sigma} \dots | 0 \rangle
 \end{aligned}$$

Need for new paradigm

- If you are interested in Neuromorphic computing or Quantum computing, drop me a line!

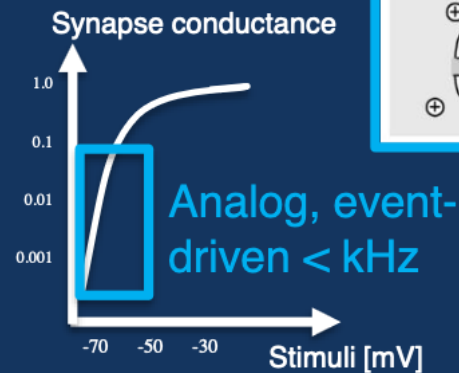
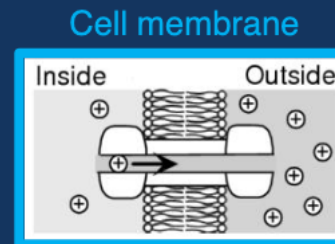
Conventional computers

mimic logical and analytical thinking

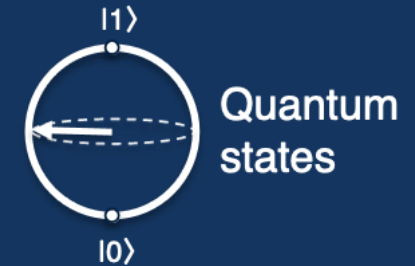


Neuromorphic processors

mimic the senses, learning and perception



Quantum processors use quantum superpositions for probabilistic inference



Technology readiness?

The MODE Collaboration

<https://mode-collaboration.github.io/>

- Joint effort
 - Particle physicists, Nuclear physicists, Astrophysicists, Computer scientists, Mathematicians
- If you are interested, join us!!!
 - Extremely loose statute, we mostly strive to talk regularly and collaborate in projects

At INFN and Università di Padova Dr. **Tommaso Dorigo**, Dr. **Pablo De Castro Manzano**, Dr. **Federica Fanzago**, Dr. **Lukas Layer**, Dr. **Giles Strong**, Dr. **Mia Tosi**, and Dr. **Hevjin Yazar**

At Université catholique de Louvain Dr. **Andrea Giammanco**, Prof. **Christophe Delaere**, and Mr. **Maxime Lagrange**
At Universidad de Oviedo and ICTEA Dr. **Pietro Vischia**

At Université Clermont Auvergne, Prof. **Julien Donini**, and Mr. **Federico Nardi** (joint with Università di Padova)

At the Higher School of Economics of Moscow, Prof. **Andrey Ustyuzhanin**, Dr. **Alexey Boldyrev**, Dr. **Denis Derkach**, and Dr. **Fedor Ratnikov**

At the Instituto de Física de Cantabria, Dr. **Pablo Martínez Ruiz del Árbol**

At CERN, Dr. **Sofia Vallecorsa**

At Karlsruher Institut für Technologie, Dr. **Jan Kieseler**

At University of Oxford Dr. **Atilim Gunes Baydin**

At New York University Prof. **Kyle Cranmer**

At Université de Liège Prof. **Gilles Louppe**

At GSI/FAIR Dr. **Anastasios Belias**

At HEPHY Vienna (OeAW) Dr. **Claudius Krause**

At Uppsala Universitet Prof. **Christian Glaser**

At TU-München, Prof. **Lukas Heinrich** and Mr. **Max Lamparth**

At Durham University Dr. **Patrick Stowell**

At Lebanese University Prof. **Haiitham Zaraket**

At University of Kaiserslautern-Landau Mr. **Max Aehle**, Prof. **Nicolas Gauger**, Dr. **Lisa Kusch**

At University of Applied Sciences Worms Prof. **Ralf Keidel**

At Princeton University Prof. **Peter Elmer**

At University of Washington Prof. **Gordon Watts**

At SLAC Dr. **Ryan Roussel**

At Lulea University of Technology Prof. **Fredrik Sandin** and Prof. **Marcus Liwicki**

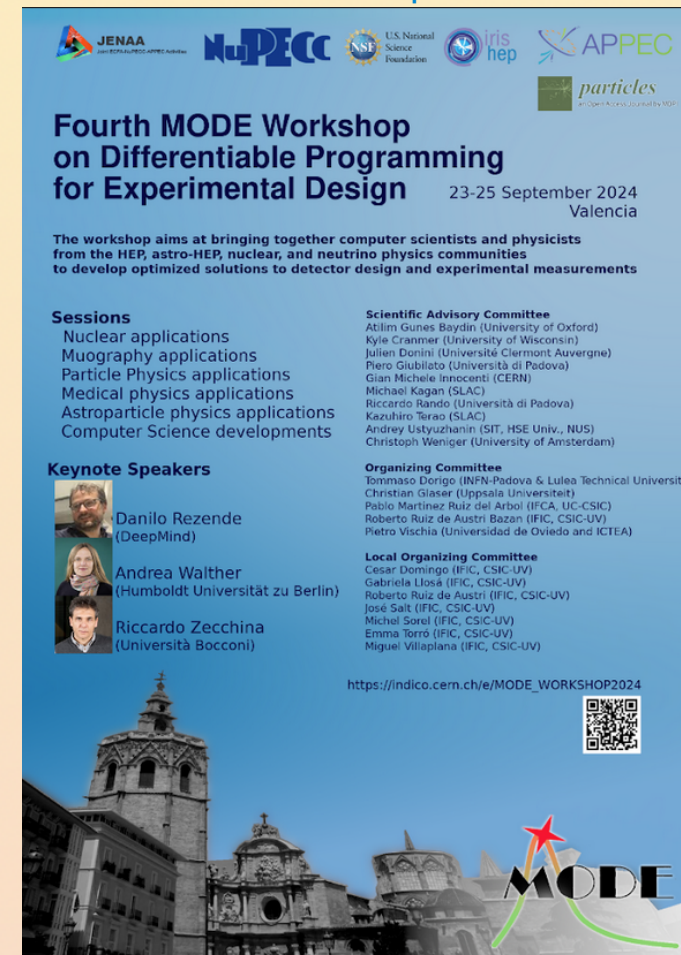
At IGFAE and Universidad de Santiago de Compostela Prof. **Xabier Cid Vidal**

The Scientific Coordinator of the MODE Collaboration is Dr. **Tommaso Dorigo**, INFN-Sezione di Padova

The Steering Board of the MODE Collaboration includes:

- Prof. **Julien Donini**, UCA
- Dr. **Tommaso Dorigo**, INFN-PD
- Dr. **Andrea Giammanco**, UCLouvain
- Dr. **Fedor Ratnikov**, HSE
- Dr. **Pietro Vischia**, UniOvi

- Come to Valencia (23-25/09/2024) for our **Fourth Workshop!!!**

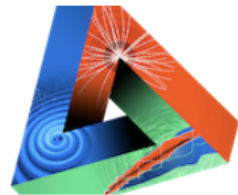


The poster for the Fourth MODE Workshop on Differentiable Programming for Experimental Design, held from 23-25 September 2024 in Valencia. It features logos for JENEA, NuPECC, NSF, US National Science Foundation, iris hep, APPEC, and particles. The workshop aims to bring together computer scientists and physicists from the HEP, astro-HEP, nuclear, and neutrino physics communities to develop optimized solutions to detector design and experimental measurements. Keynote speakers include Danilo Rezende (DeepMind), Andrea Walther (Humboldt Universität zu Berlin), and Riccardo Zecchina (Università Bocconi). The poster also lists the Scientific Advisory Committee, Organizing Committee, and Local Organizing Committee. A QR code and the URL https://indico.cern.ch/e/MODE_WORKSHOP2024 are provided. The background of the poster shows a photograph of a historic building in Valencia.

European AI structures

- European initiative for advancing the use of AI in Fundamental Physics: <https://eucaif.org>
 - The [First EuCaif conference](#) took place in Amsterdam beginning of May
 - [Work Package 2: Experiment Design](#)

EUROPEAN COALITION FOR AI IN
FUNDAMENTAL PHYSICS



JENAA

Joint ECFA-NuPECC-APPEC Activities

Thank you!



Backup

From POCA to extended POCA

- POCA (POint of Closest Approach) assumes one scattering in one point \rightarrow bias
 - invert model to compute X_0 , then average X_0 per voxel
- Extend to nearby bins within uncertainty
 - Extrapolated from track uncertainty from analytical fit
- Assume one scattering \rightarrow bias!

