The MODE Collaboration Effort

Jan Kieseler

3.3.2022

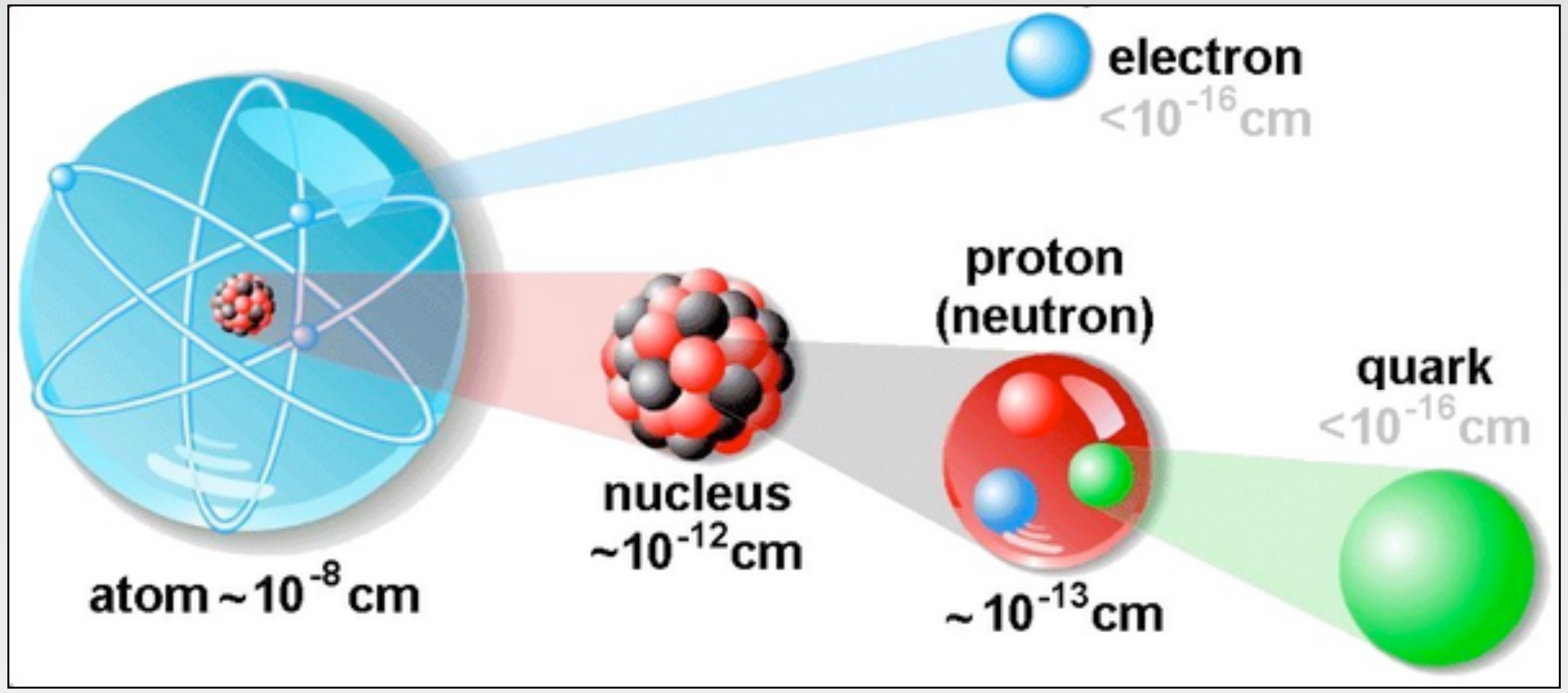
- selected topics -

Machine-Learning **O**ptimised **D**esign of **E**xperiments
https://mode-collaboration.github.io

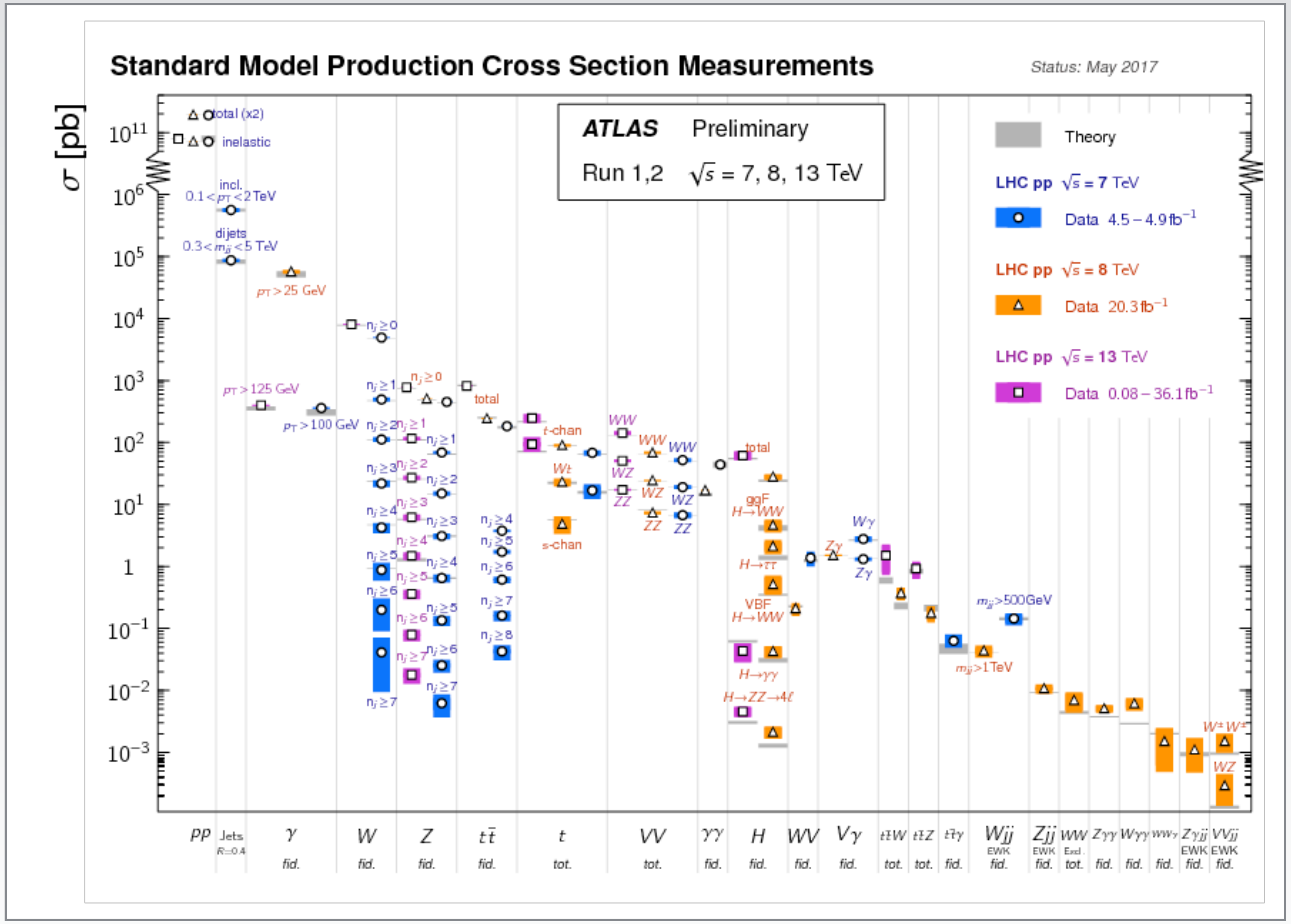
At University of Padova Dr. **Tommaso Dorigo**, Dr. **Pablo De Castro Manzano**, Dr. **Lukas Layer**, Dr. **Giles Strong**, Dr. **Mia Tosi**, and Dr. **Hevjin Yarar**
At Université catholique de Louvain Dr. **Andrea Giammanco**, Prof. **Christophe Delaere**, Mr. **Maxime Lagrange**, and Dr. **Pietro Vischia**
At Université Clermont Auvergne, Prof. **Julien Donini**, and Mr. **Federico Nardi**
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 Ruíz del Árbol**
At CERN Dr. **Lukas Heinrich** and 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 Dr. **Anastasios Belias**
At Rutgers University Dr. **Claudius Krause**
At Uppsala Universitet Prof. **Christian Glaser**
At TU-München Mr. **Max Lamparth**
At Durham University Dr. **Patrick Stowell**
At Lebanese University Prof. **Haitham Zaraket**

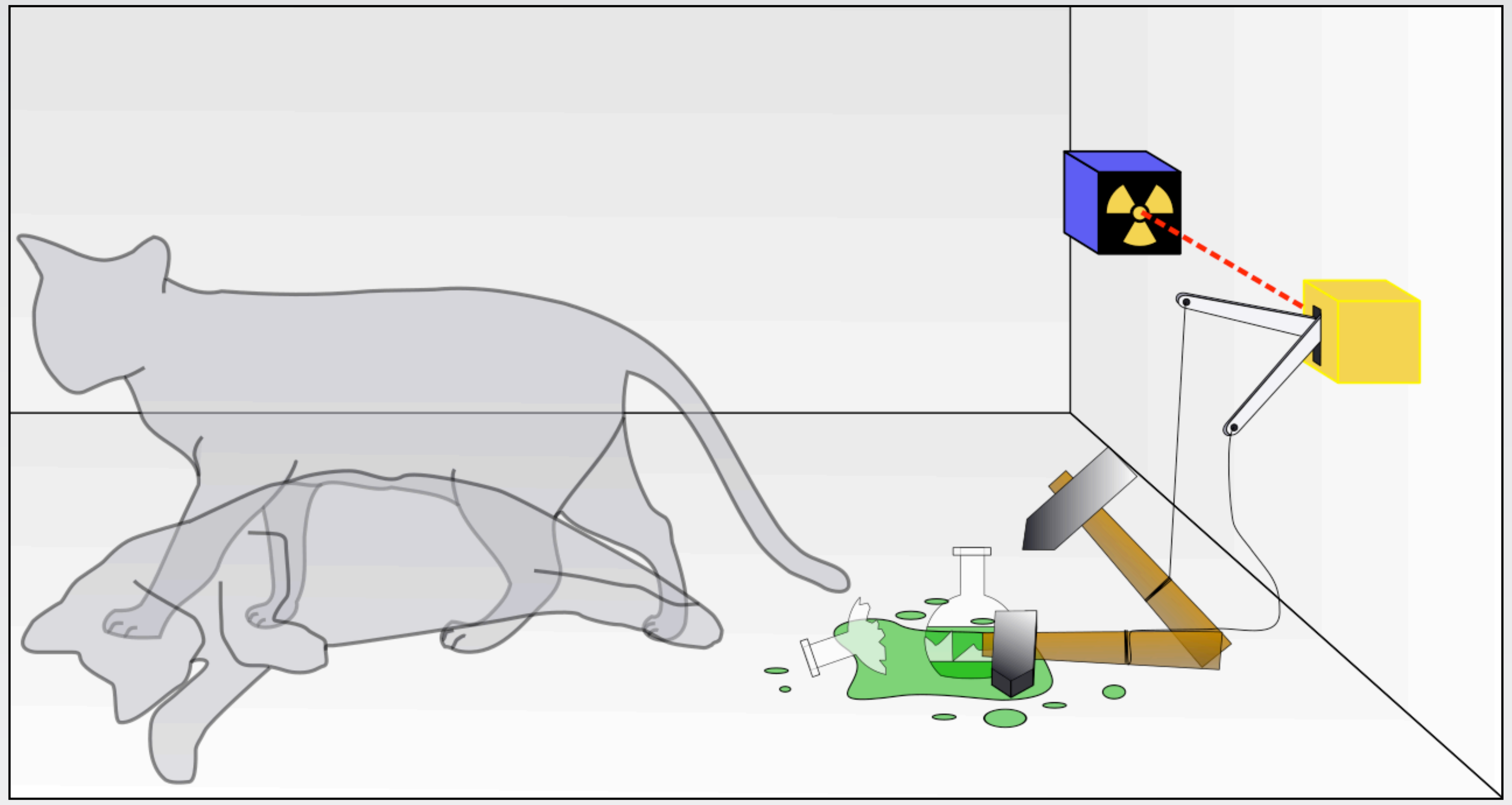
What are we looking for?

- Dark matter
- Stability of the universe
- Grand unifying theories
- Resolution ~ energy



Underlying Model

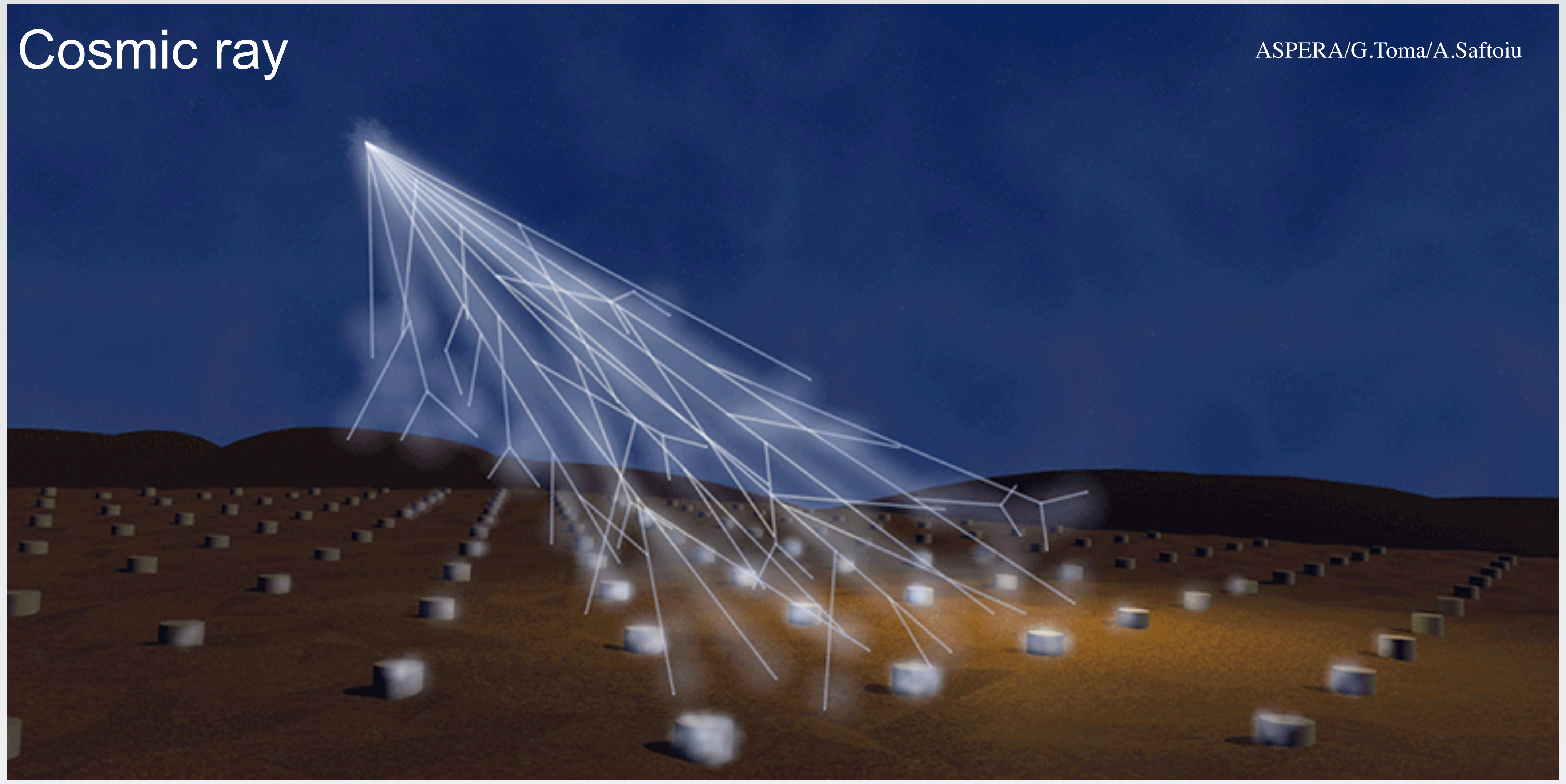


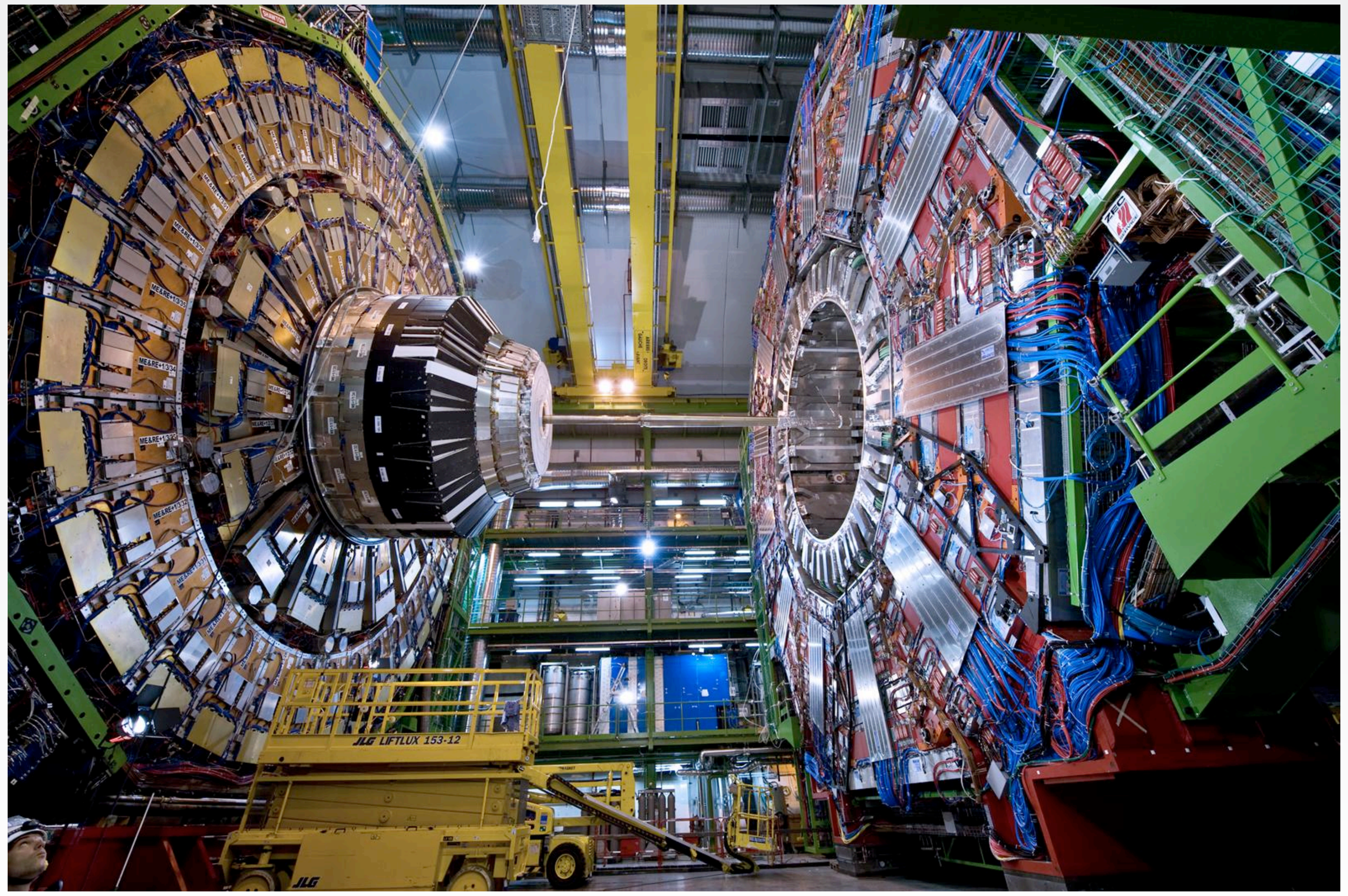


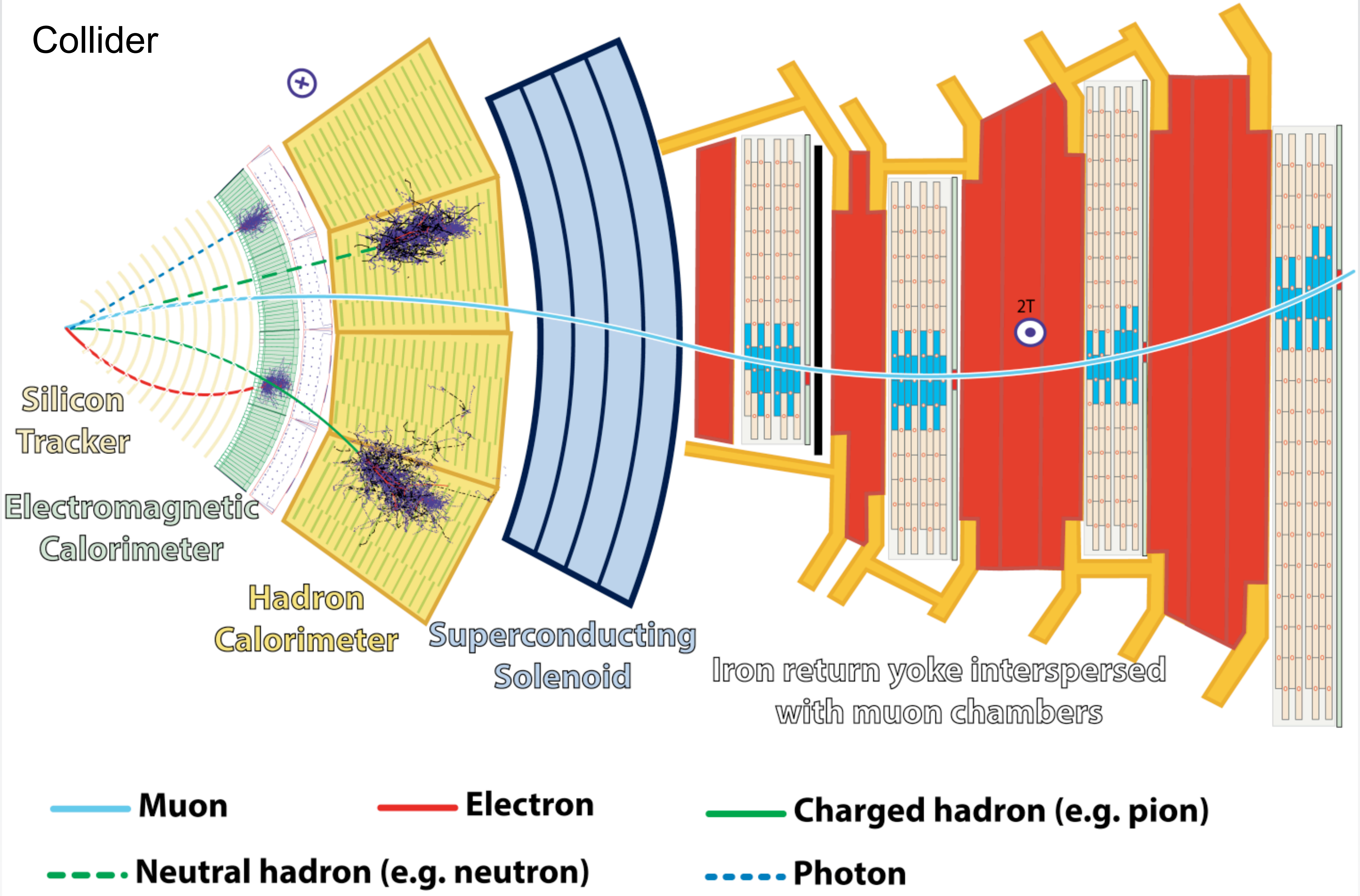
By Dhatfield - Own work, CC BY-SA 3.0,
https://commons.wikimedia.org/w/index.php?curid=4279886

- Remarkable theory
  - spanning order of magnitude
  - precision predictions
- Stochastic in nature
- Go deeper: new, more powerful colliders

Detect Particles and Processes

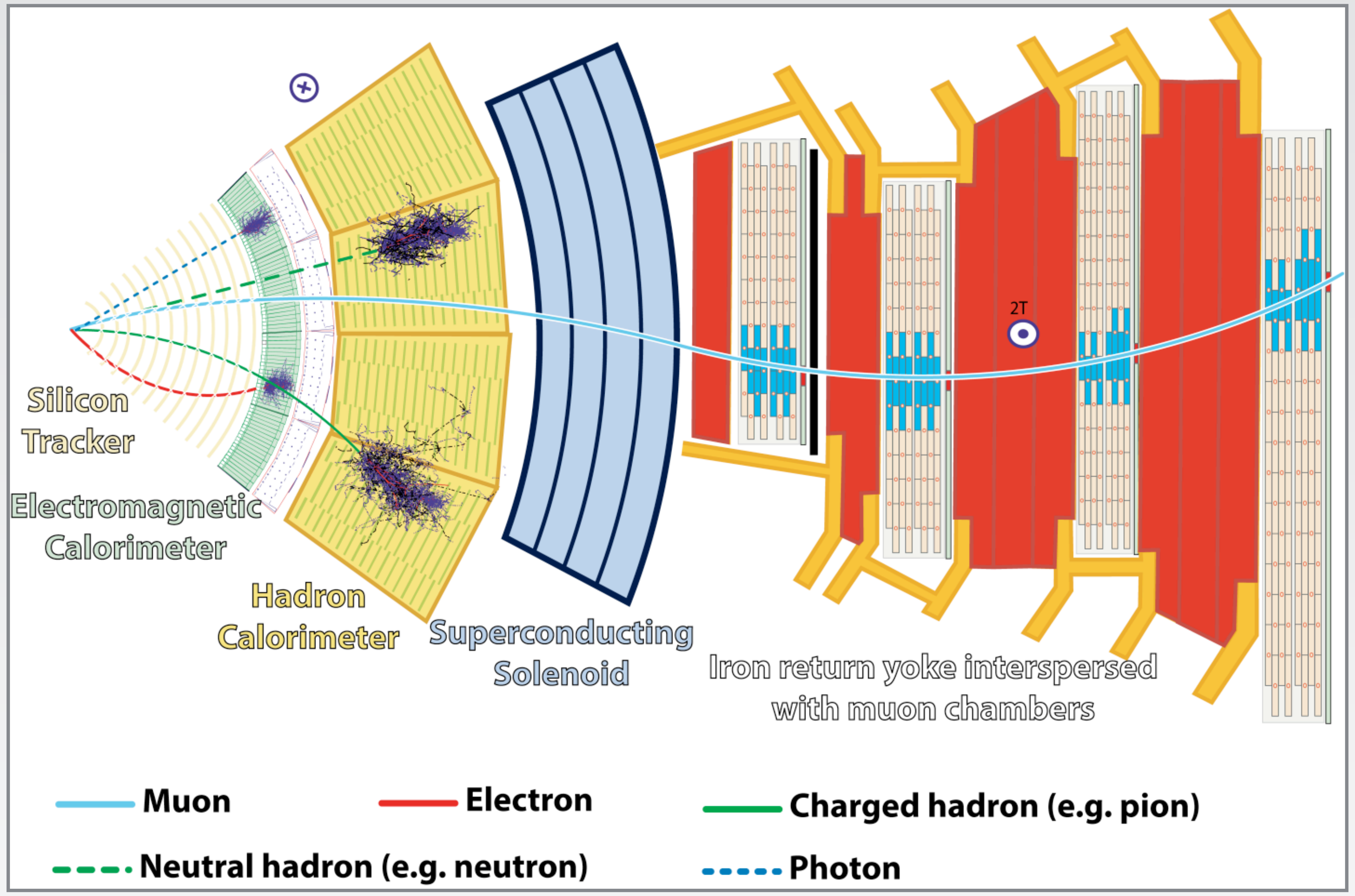


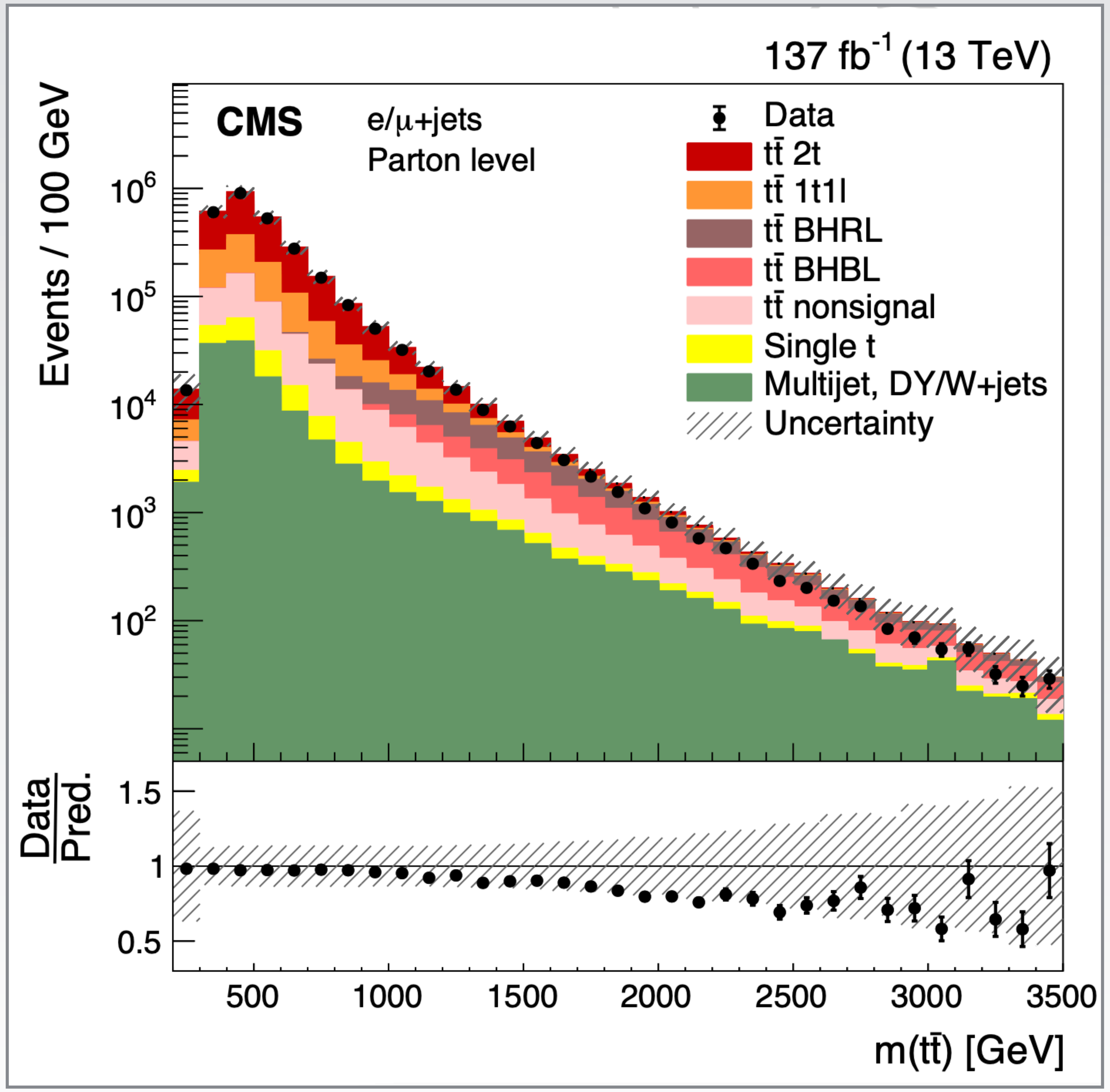




- We measure decay products of the stochastic process
- Detectors employ parts of or all of the above concepts

Simulation of detector response



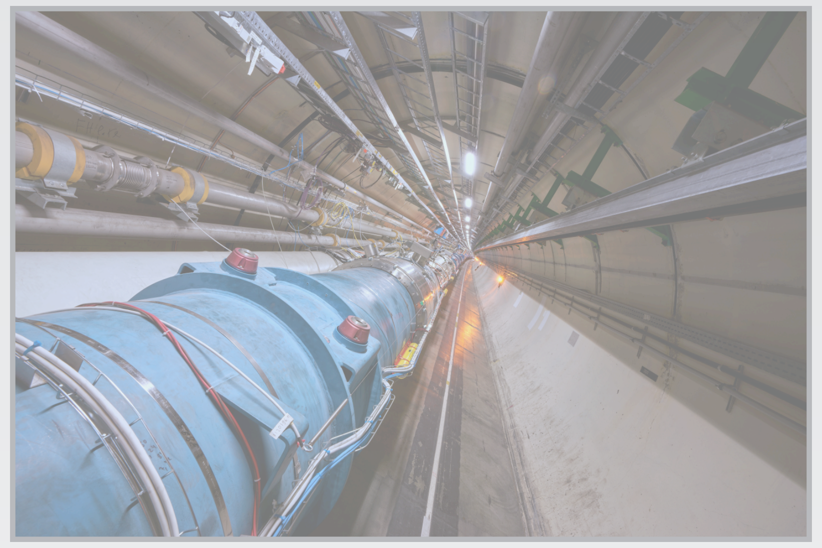


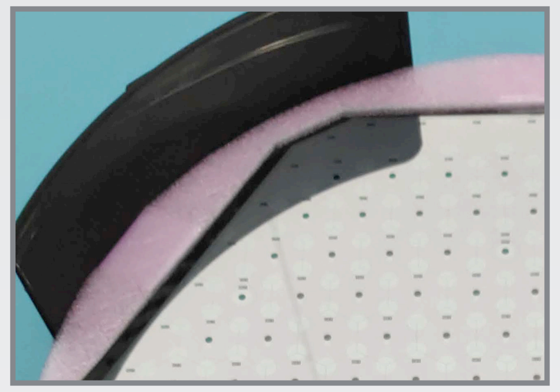
http://arxiv.org/abs/2108.02803

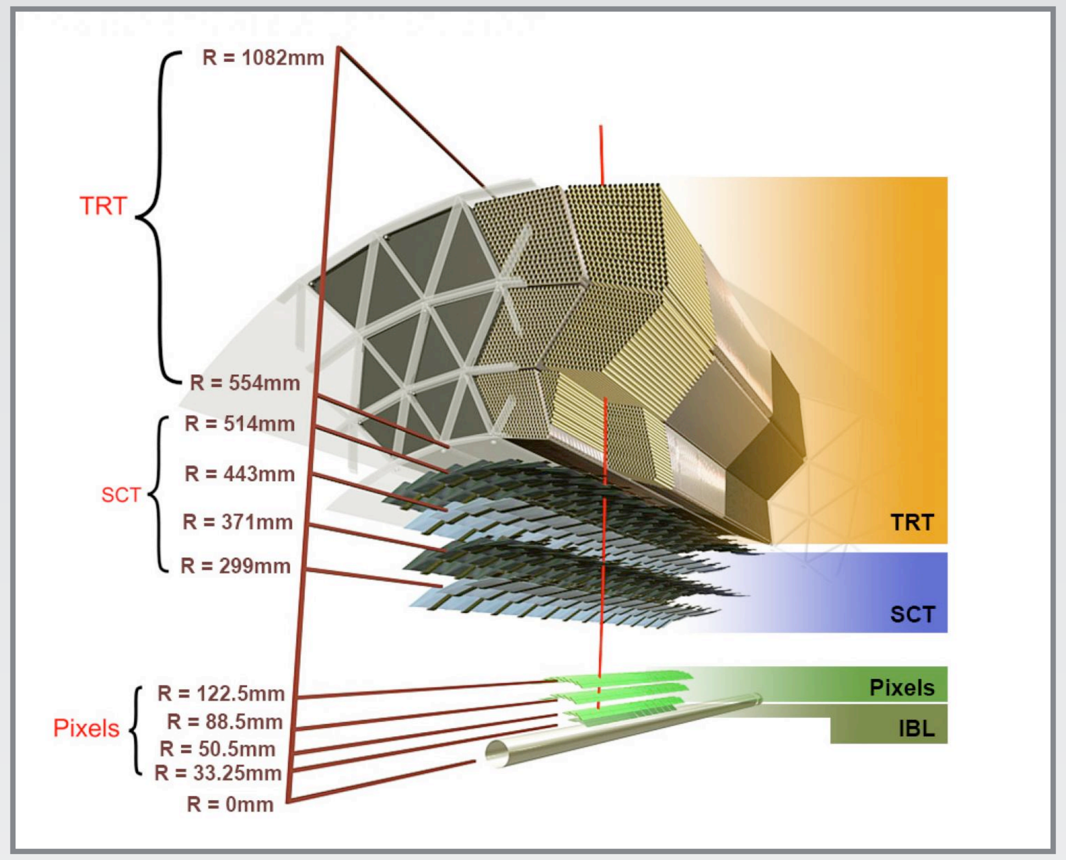
- High fidelity simulation of particles interacting with matter
- Carefully validated

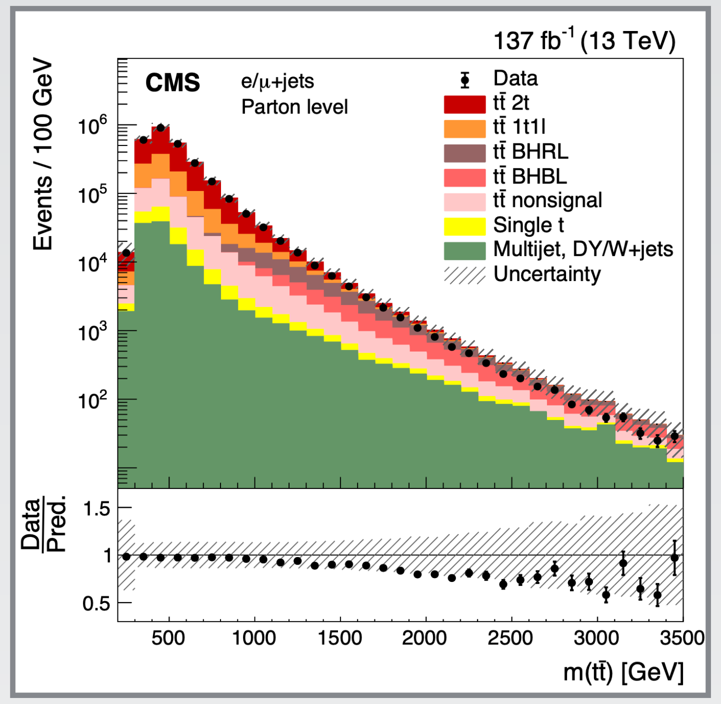
- Validity also spans orders of magnitude

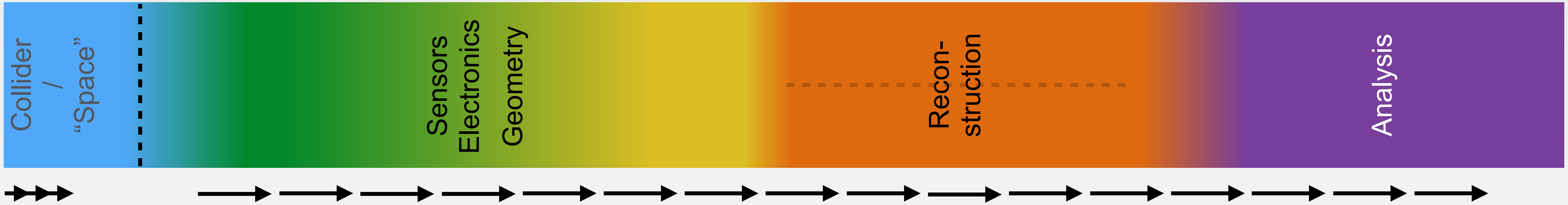
The status quo

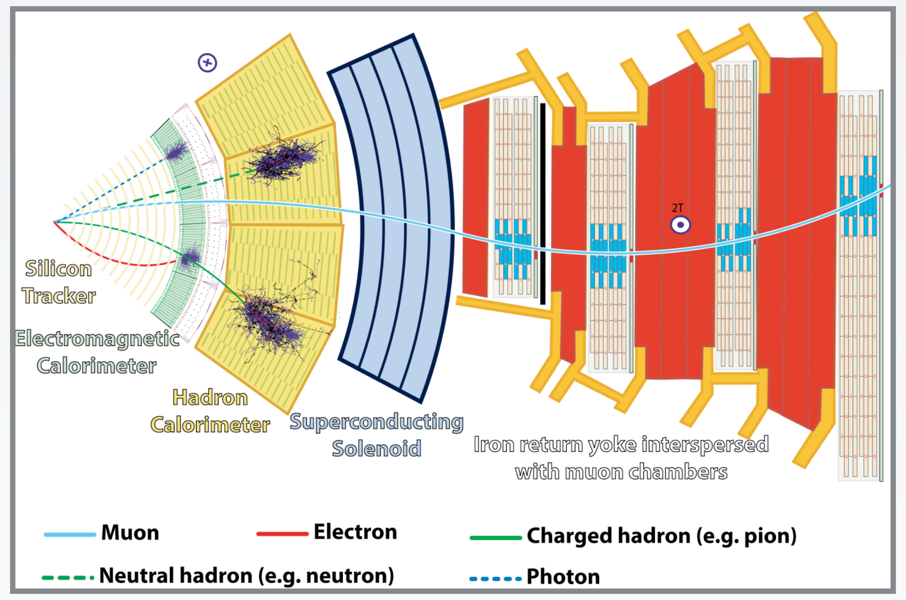


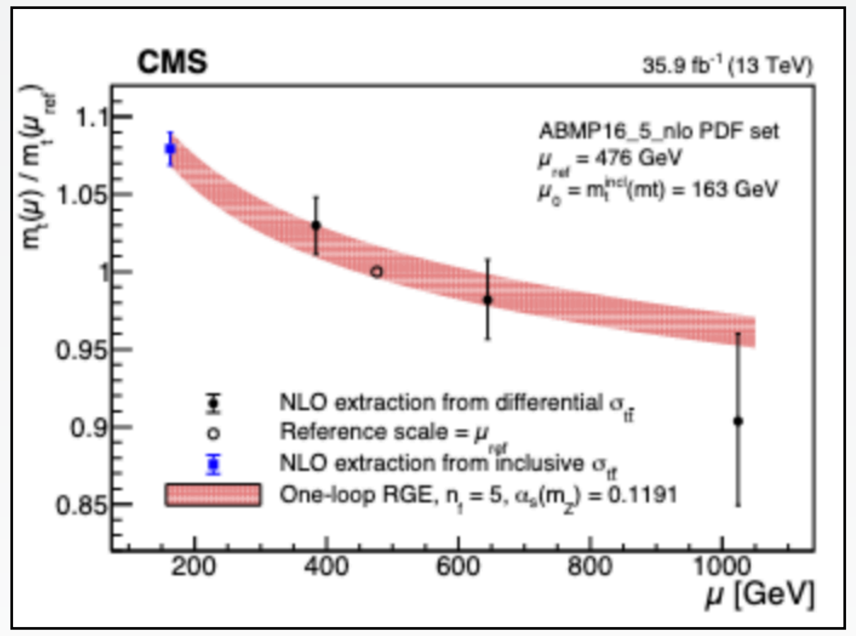












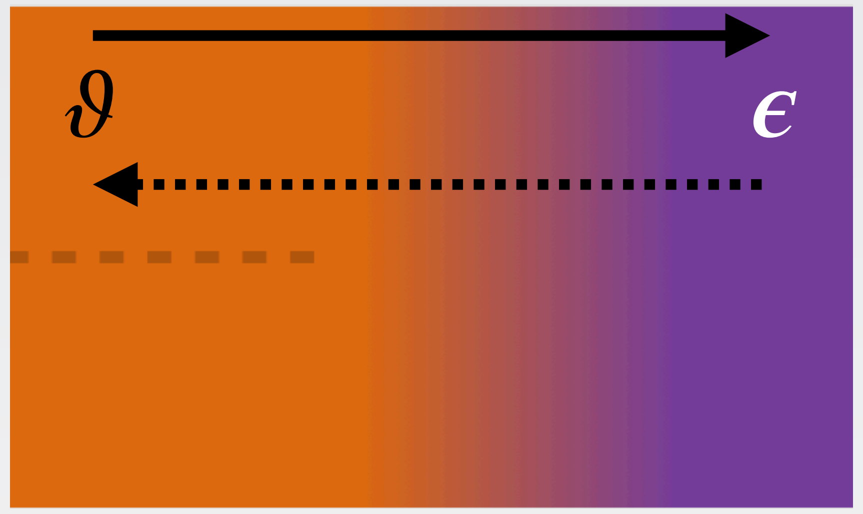
arXiv:1909.09193

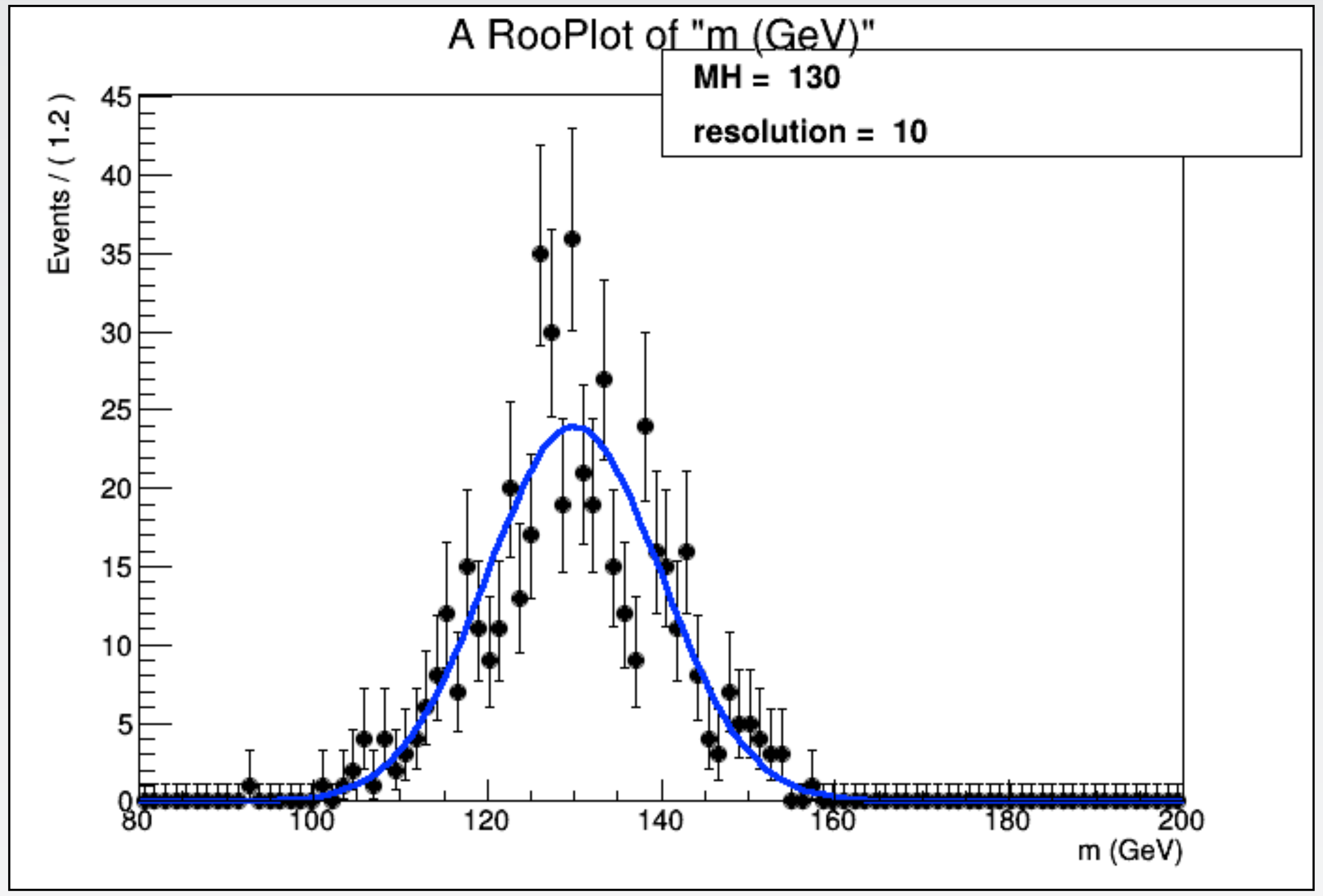
- Very high dimensional parameter space
- An expert group at each step
  - Very well-understood steps
  - Use surrogates and short cuts to the final objective (physics result)
  - The chain has **almost no parts** expressed in a differentiable way (or code)
  - **Tuning often by hand** and optimisations take a lot of time and person power

Determining multiple parameters

- Determining multiple parameters ~ fitting a function

- The optimisation of a detector or a reconstruction chain is conceptually the same thing





- To perform this optimisation we need to know $\partial\epsilon/\partial\vartheta$: how does our photon efficiency change w.r.t. the reconstruction parameters ϑ?

- Gradients can be calculated
  - Numerically: unfeasible for many parameters
  - Algorithmically: requires *unbroken* gradients throughout the whole chain: every step needs to be differentiable

  ➡ Differential programming

Interlude: differentiable programming in a 

- Differentiable programming is used by, but is independent of machine learning.

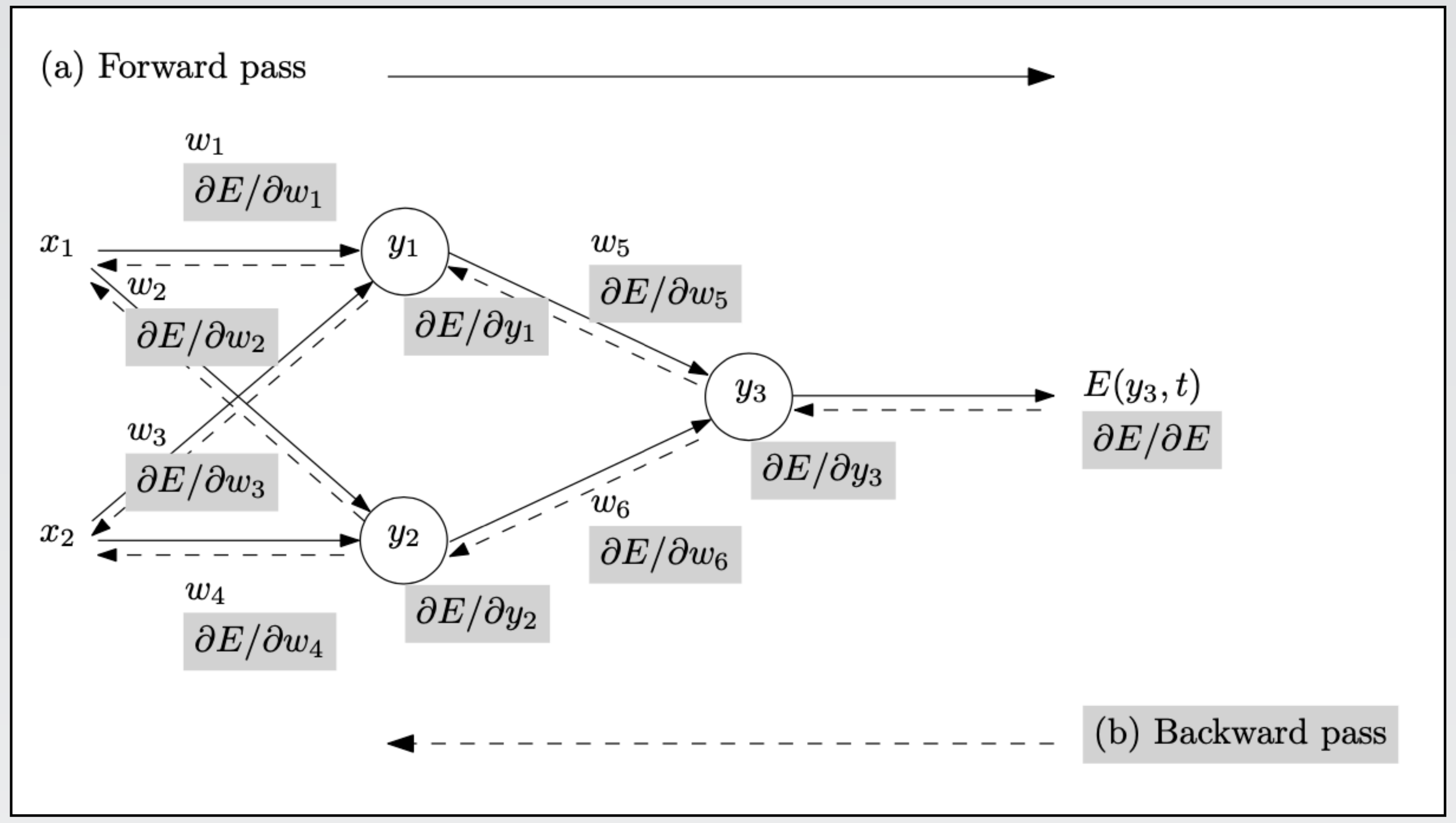
- At its core: in any operation, include a way to access its gradient w.r.t. all parameters (if it exists): auto differentiation

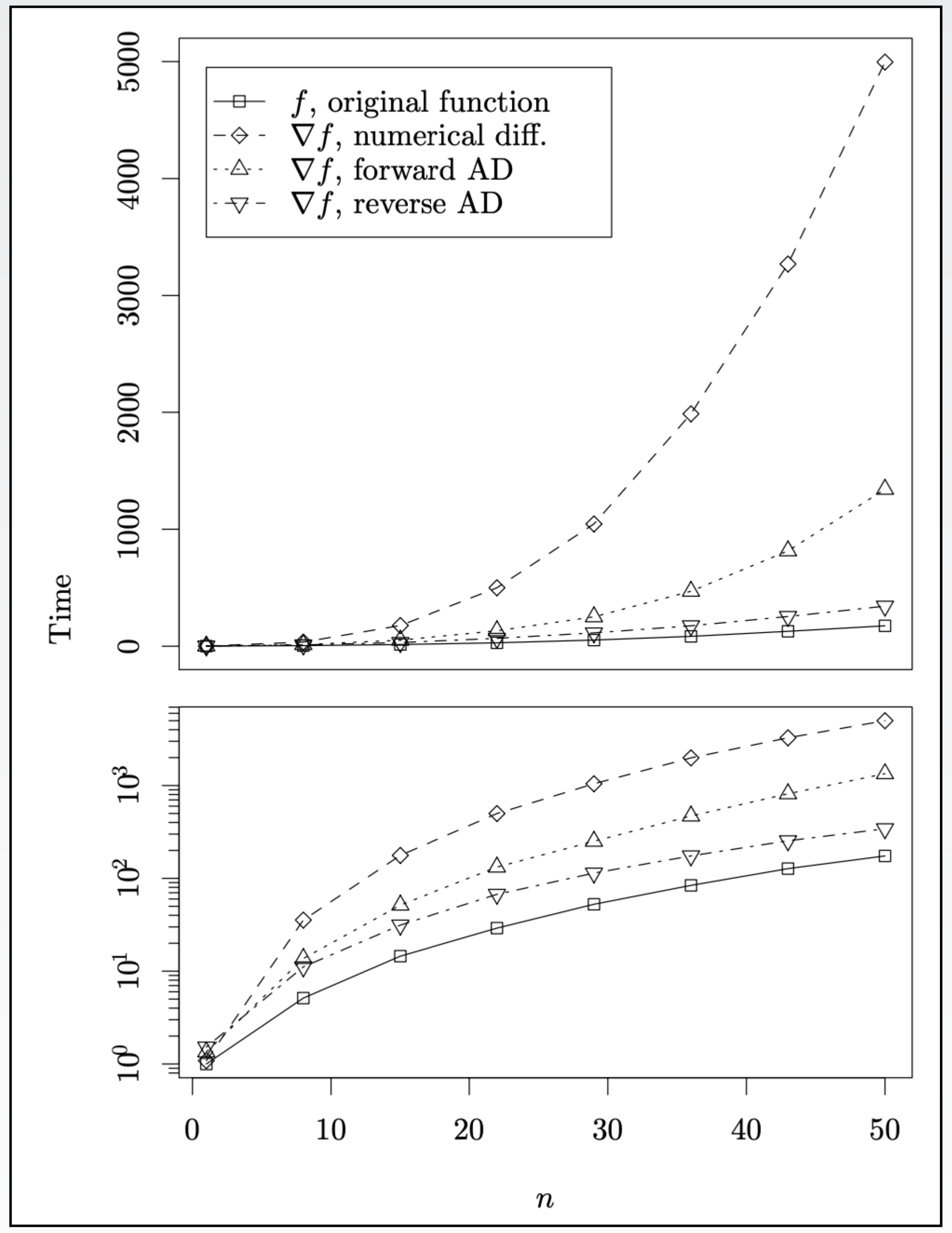
- Auto-differentiation is neither pure numeric nor pure symbolic differentiation
  - Numerical differentiation is not feasible for large optimisation problems
  - Fully symbolic differentiation can easily become not feasible from computational point of view

- In most cases, back propagation is used
  dL/dA = dx/dA dL/dx   A → x → L
  - Calculate the numerical values of b = dL/dx using the analytic gradient of the operation
  - Calculate the numerical values of b * dx/dA in the same way

- Each ‘atomic’ simple operation only needs to be equipped with a simple analytic gradient, then evaluated numerically: best of both worlds.

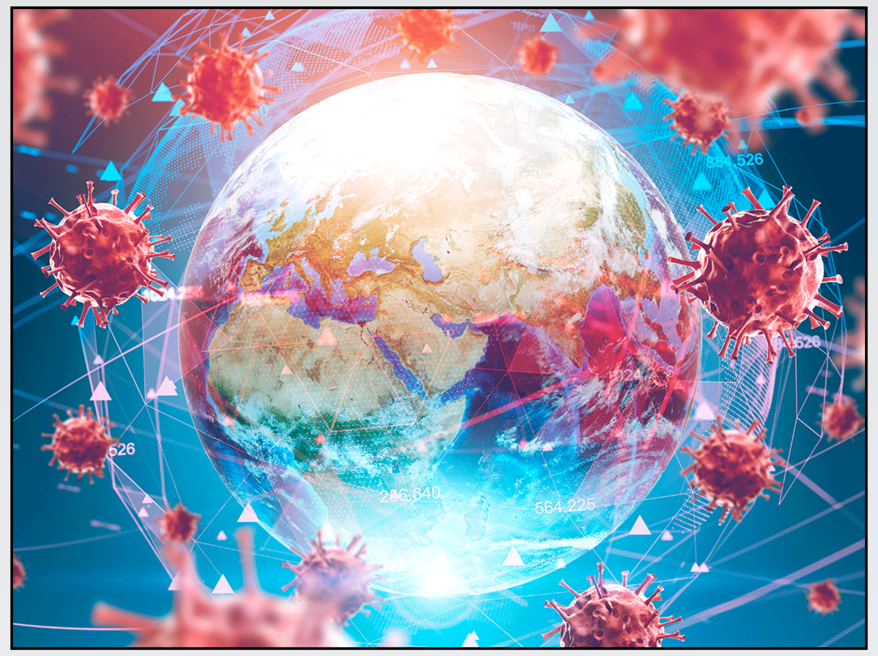
- This is implemented in one way or another in all modern ML frameworks (TF, torch..)
- *Even expressing non-ML algorithms in differentiable frameworks comes with huge advantages w.r.t. the capability of optimising their parameters, and using state-of-the-art libraries to do so*

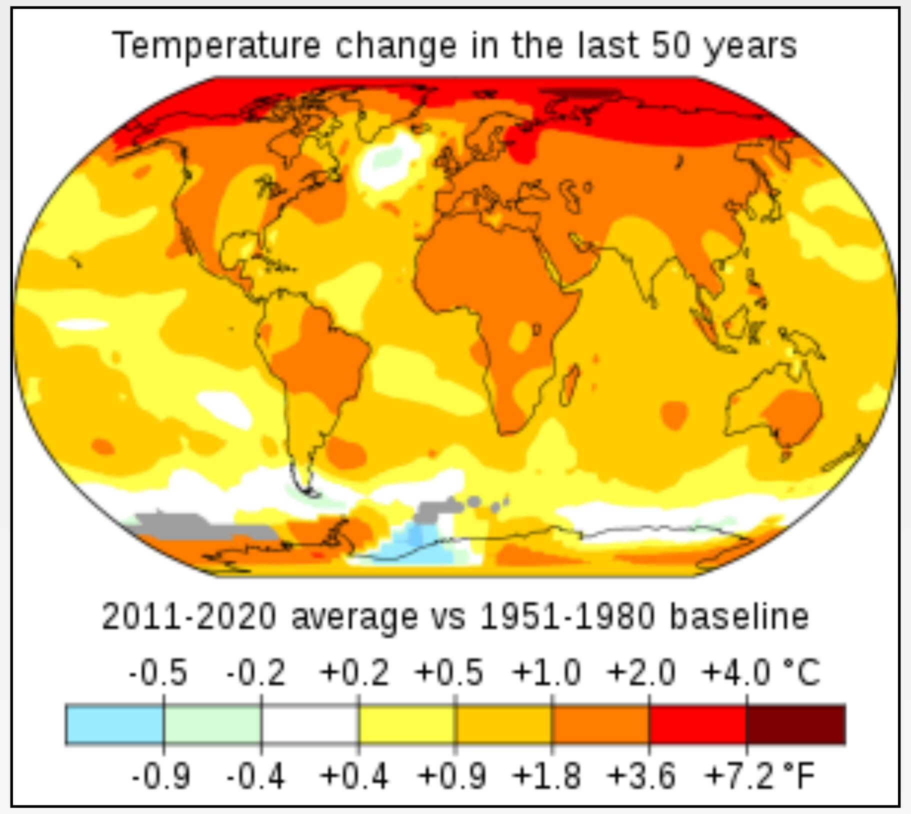




For a nice overview see Atılım Günes Baydin et al (2018), arXiv:1502.05767v4

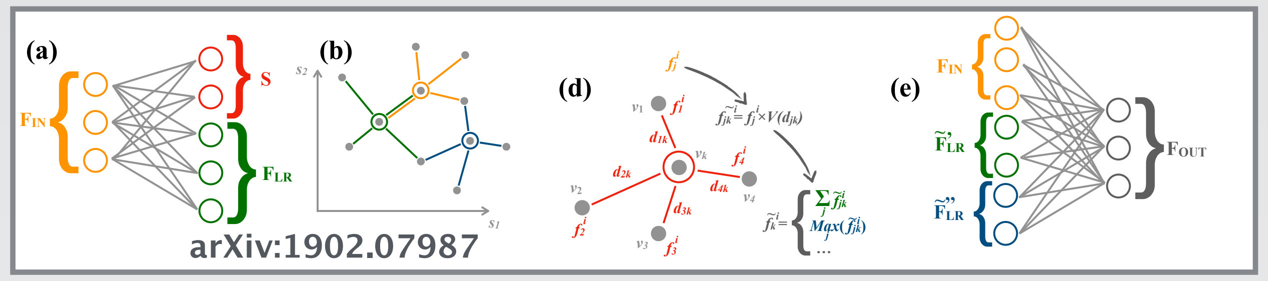
The MODE Collaboration: Goals



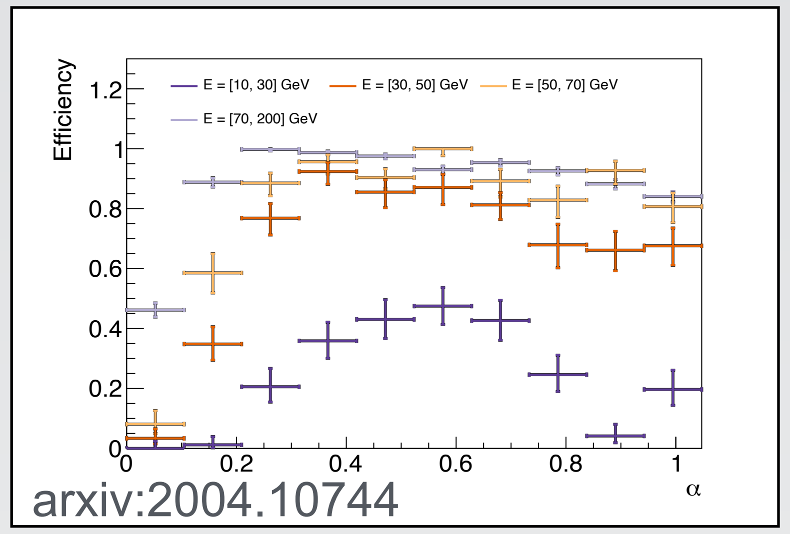


Use differentiable programming to optimise particle physics detectors given a quantification of the physics target(s) and the detector cost

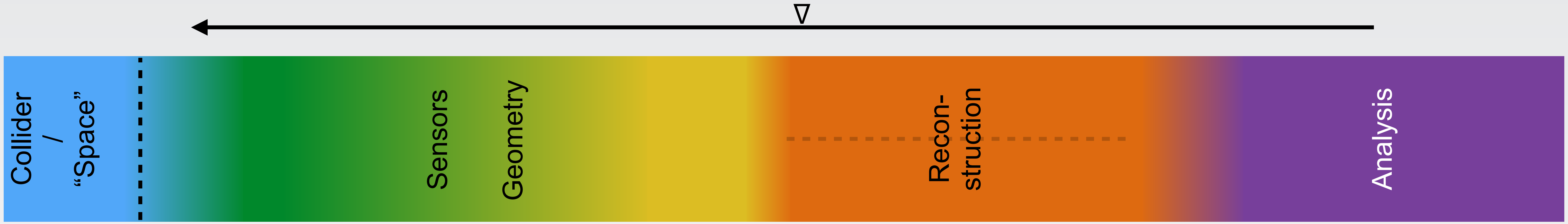
What do we already have

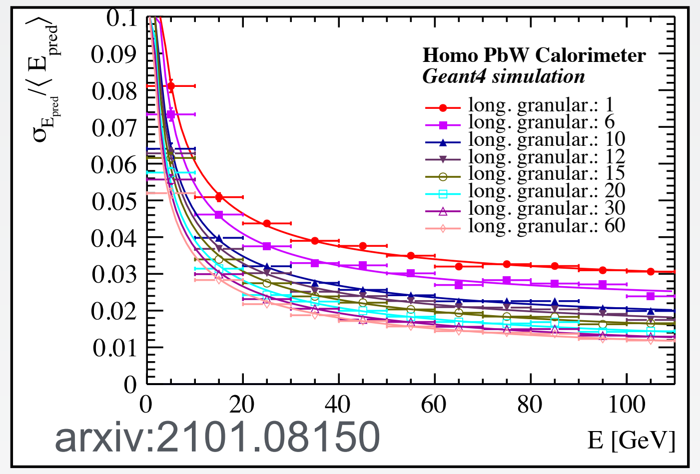


arXiv:1902.07987

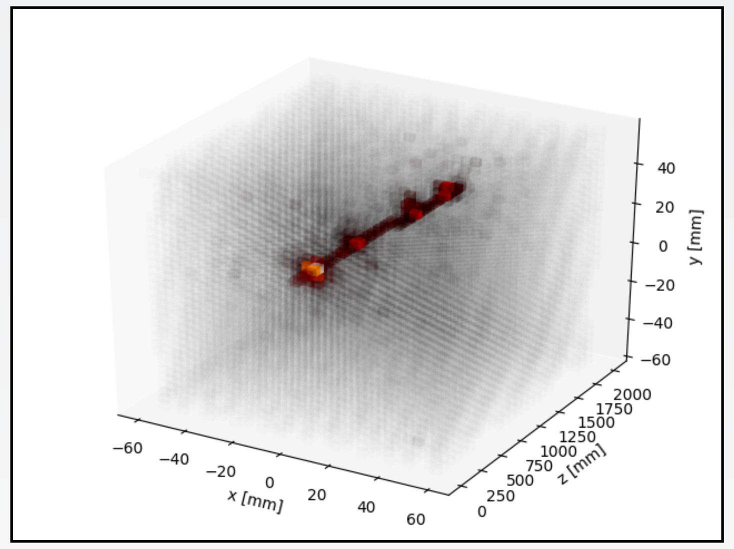


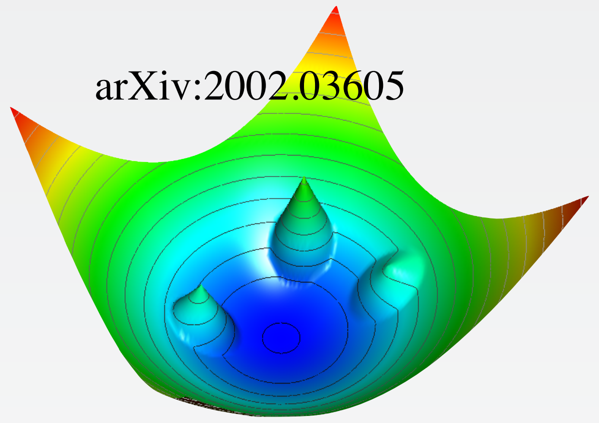
arxiv:2004.10744

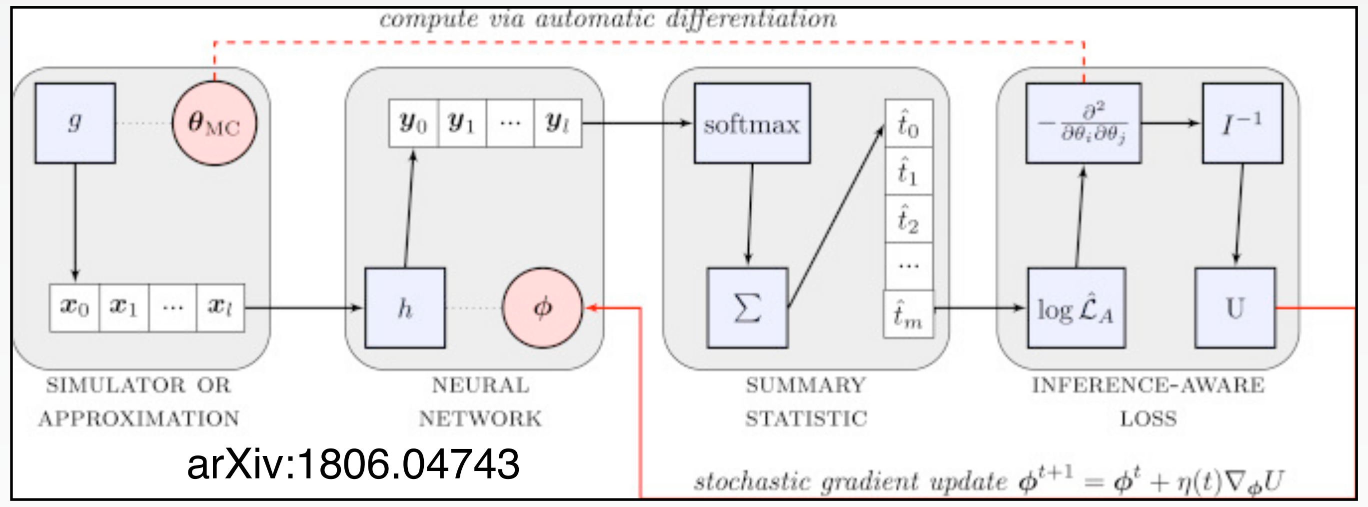




arxiv:2101.08150

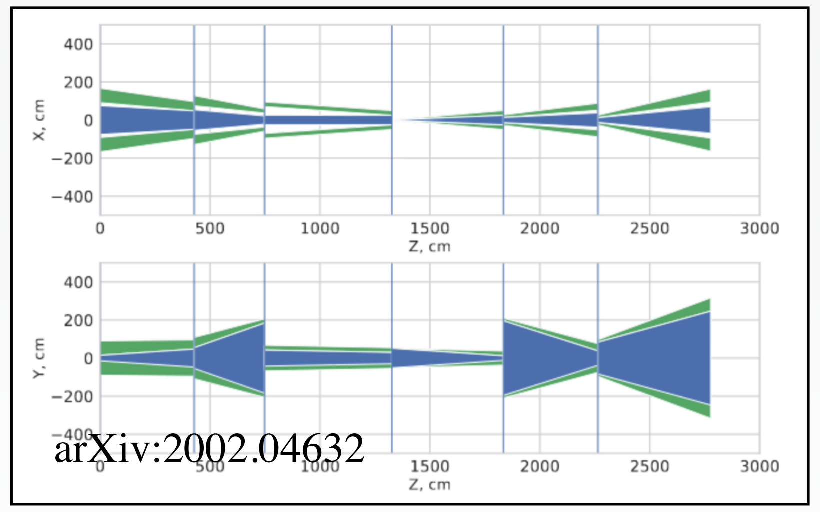



arXiv:2002.03605



arXiv:1806.04743

- Proofs of concept (or more) exist
- Overarching connection is missing
- Next: will be going backwards



arXiv:2002.04632

A typical high-energy physics analysis

Data

- Includes the full chain up to final state particle reconstruction

Simulation

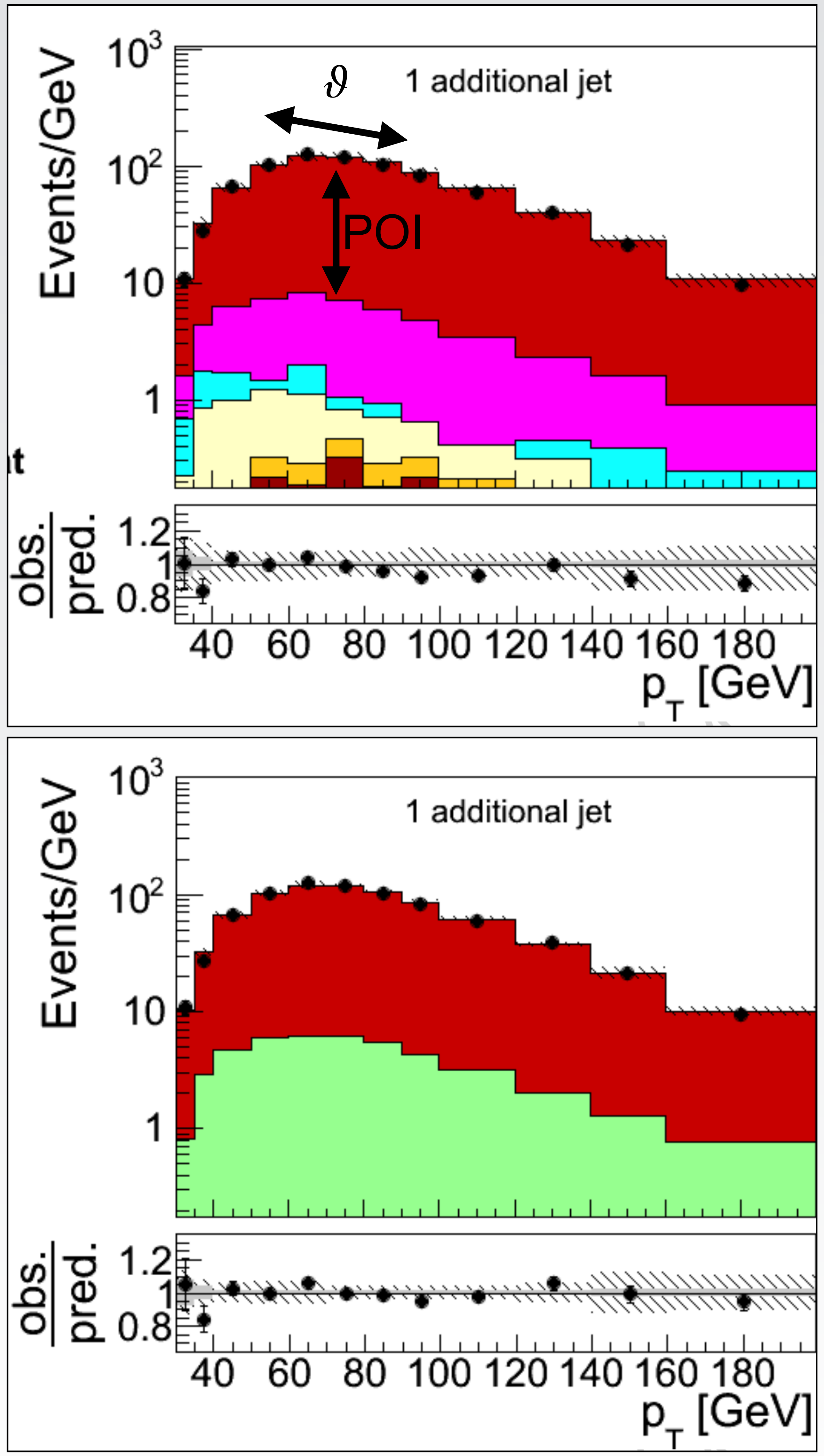
- Simulate different physics processes
- Simulate detector response and electronics
- Proceed as for data
- Calibrate and correct using control samples in data
- *Assign uncertainties on normalisation and shapes*

Analysis

- Create histograms of data and simulation
- A contribution of a process or a shape to the data: **signal**
- Contributions of other processes: **background**

- Perform profile likelihood fit of parameters of interest and parameters representing variations w.r.t. uncertainties

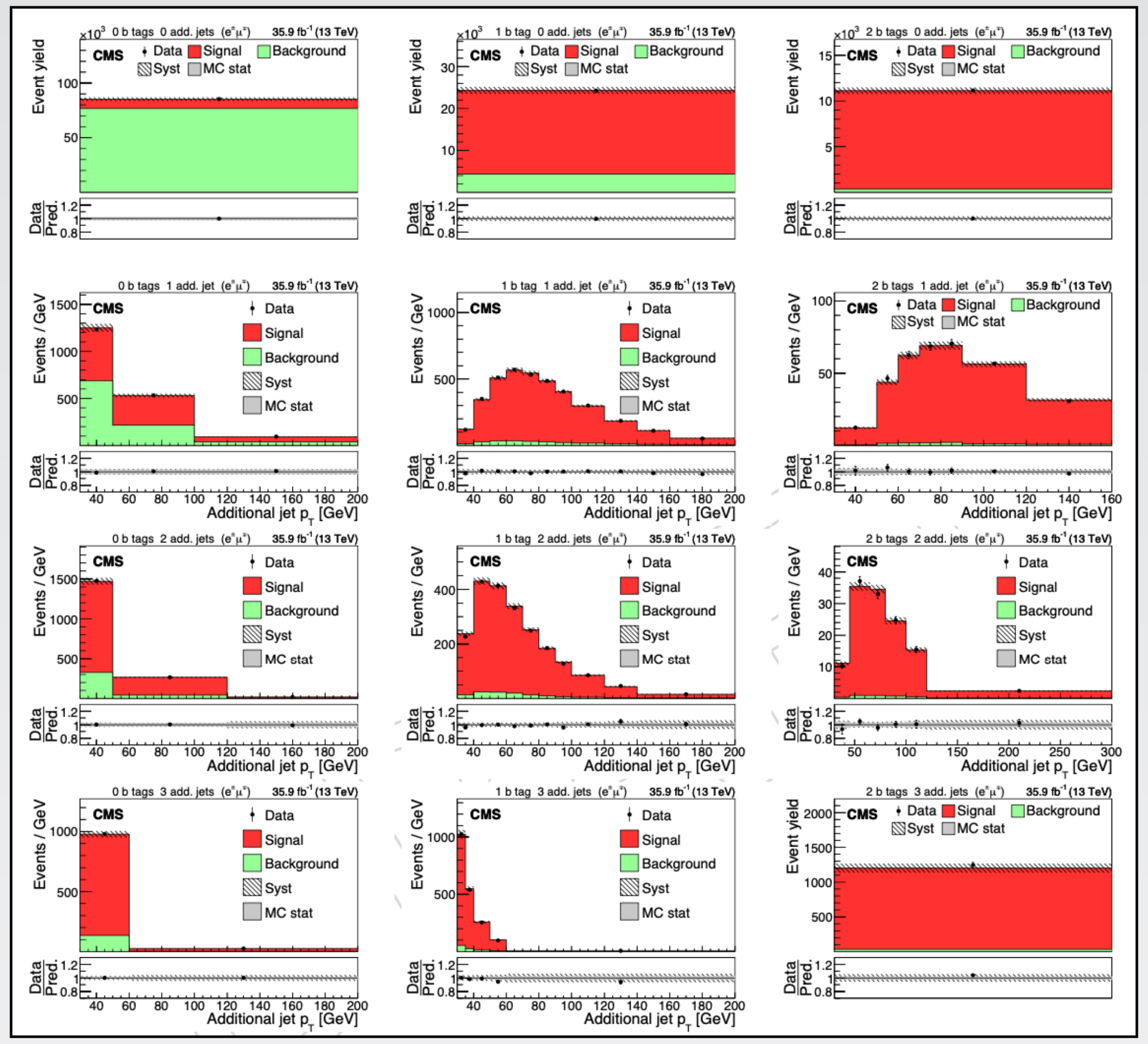
Uncertainties can be (significantly) reduced by choosing good observables to fit



CMS, arXiv:1603.02303

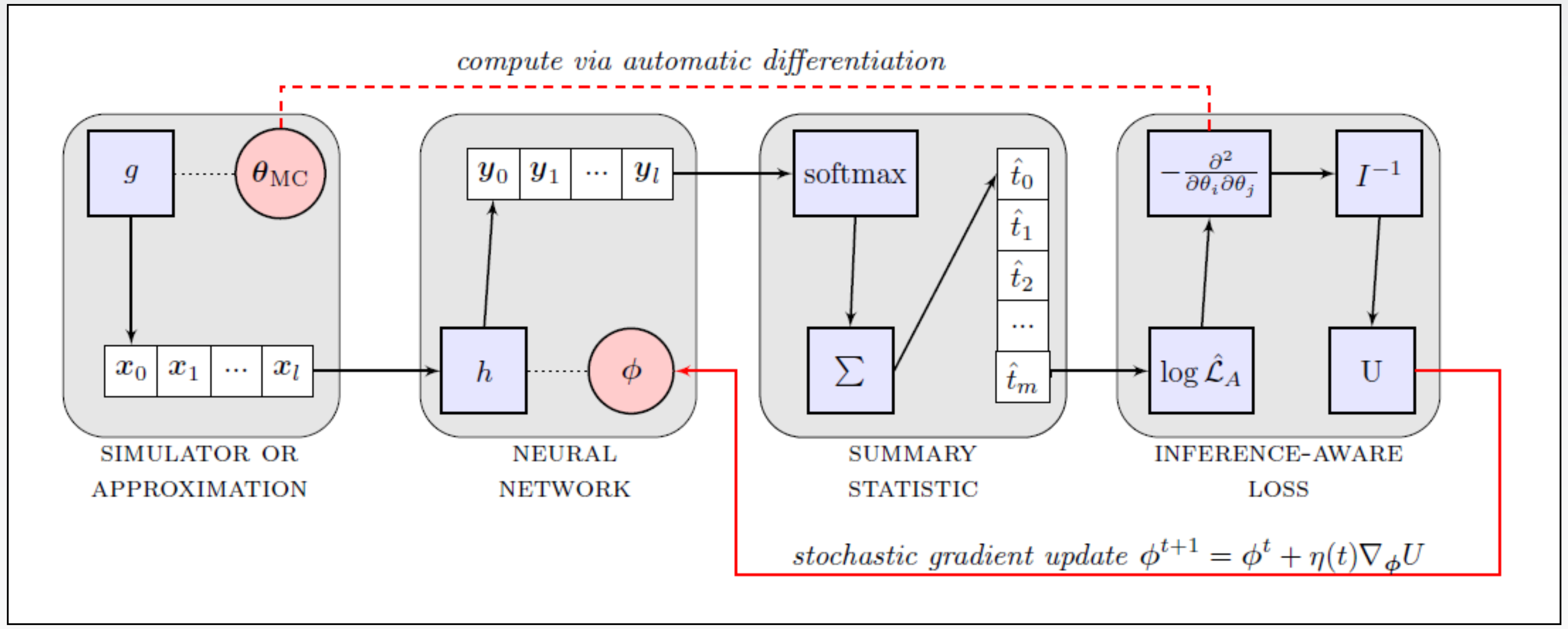
Automatising analyses on simulation

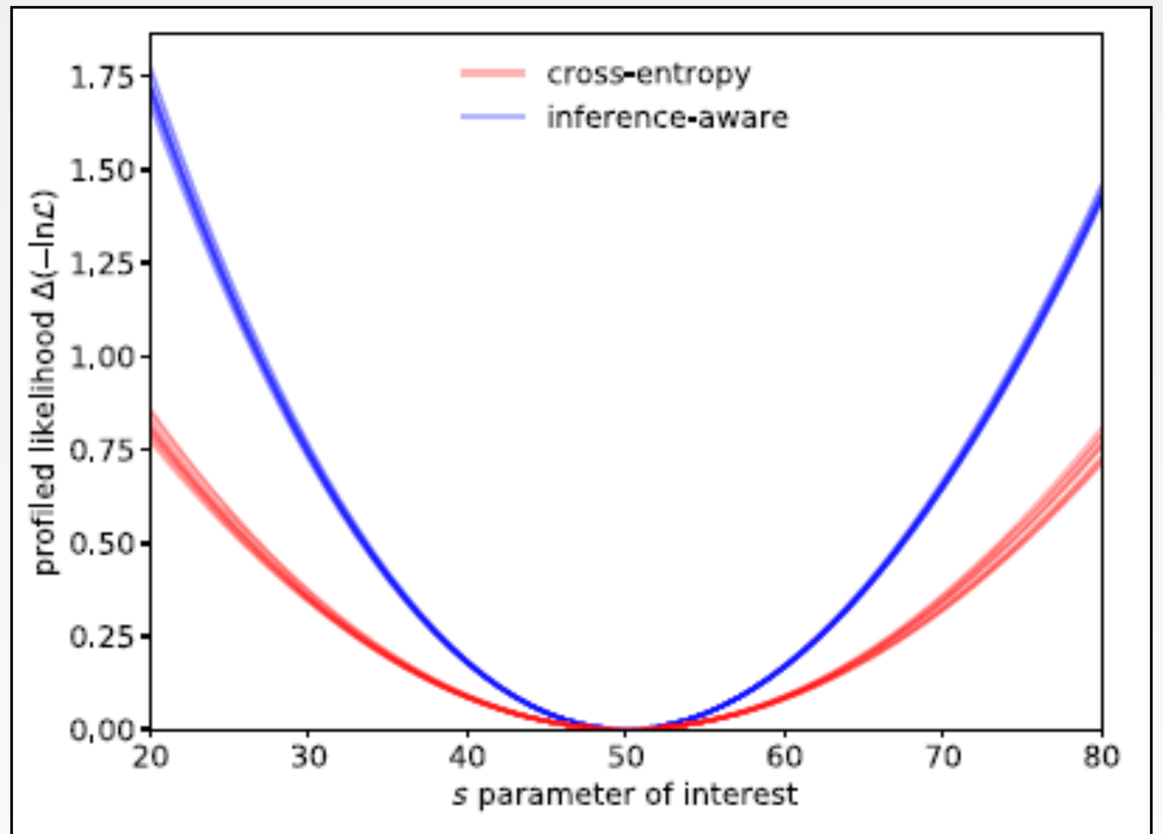
- Standard analysis concept: perform fit to data based on histograms
  - Best signal fraction (S/S+B)
    - Often use a trained classifier here
  - Lowest uncertainties



- Can take into account uncertainties in to learn not only best S/S+B, but also lowest uncertainty: INFERNO [2]

- Derive “best histogram” and perform a standard profile likelihood fit to extract the physics result





(b) profile-likelihood comparison

✓Concepts for generalisable, differentiable analyses workflows exist

Other methods overview in Bremer, Cranmer et al, arXiv:1911.01429

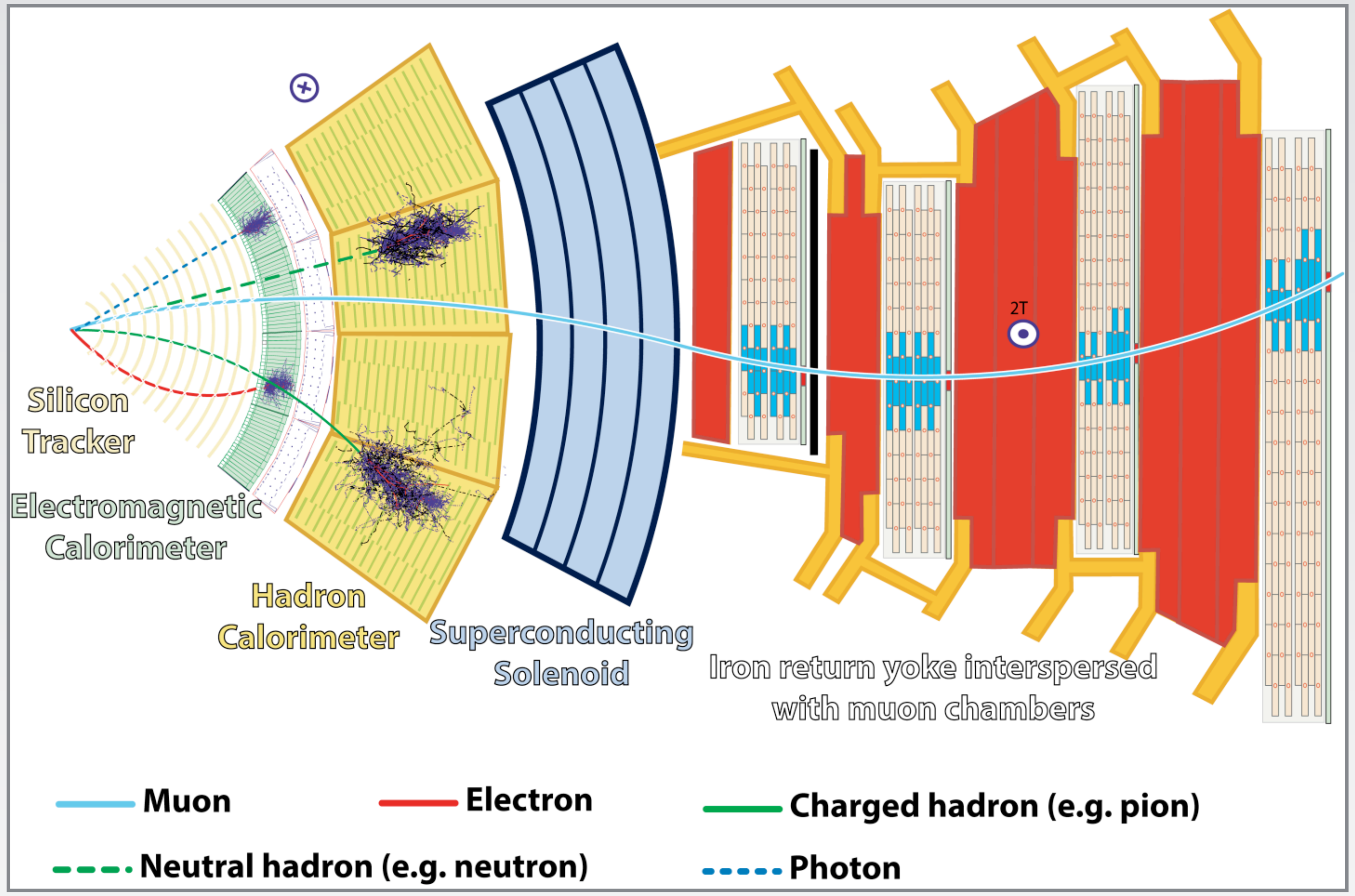
[2] P. Castro, T. Dorigo, arxiv:1806.04743v2

- Determine final state particles and their properties from detector hits

The usual chain
- Local seeding (pattern recognition)
- Local clustering (pattern recognition)
- Software compensation (pattern recognition)
- Identification (pattern recognition)
- Linking of individual detector parts (pattern recognition)

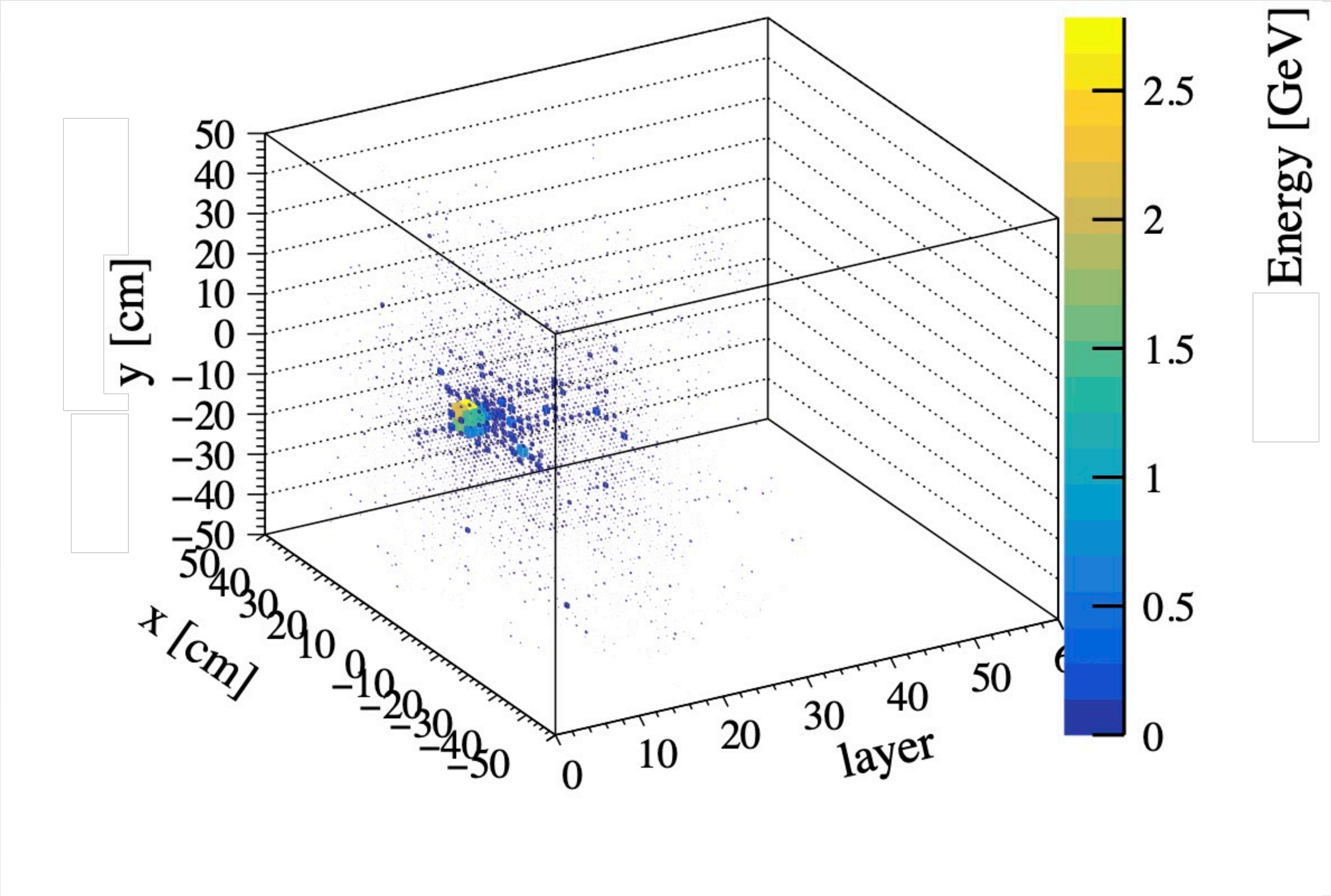
Always the same patterns

Many steps cutting / segmenting information: a priori non differentiable

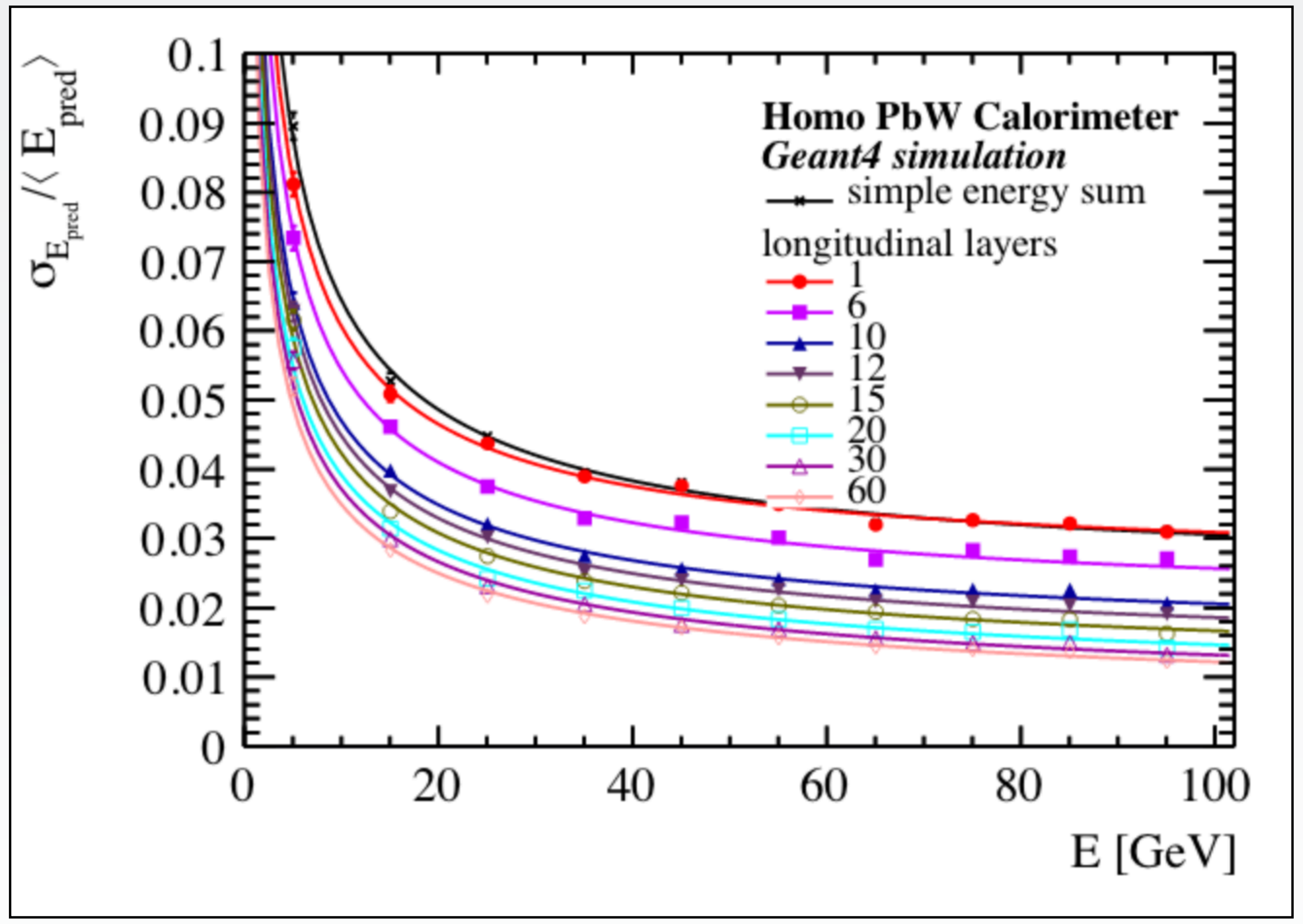


Use DNNs as generic reconstruction

The usual chain
- Local seeding (pattern recognition)
- Local clustering (pattern recognition)
- Software compensation (pattern recognition)
- Identification (pattern recognition)
- Linking of individual detector parts (pattern recognition)



- Use ML for the task: CNN structure
  - Adapts itself to grid-like granularity
  - Re-optimisation == a few GPU hours vs. months of optimisations by hand
- Compare different segmentations
  - Saturation effects visible

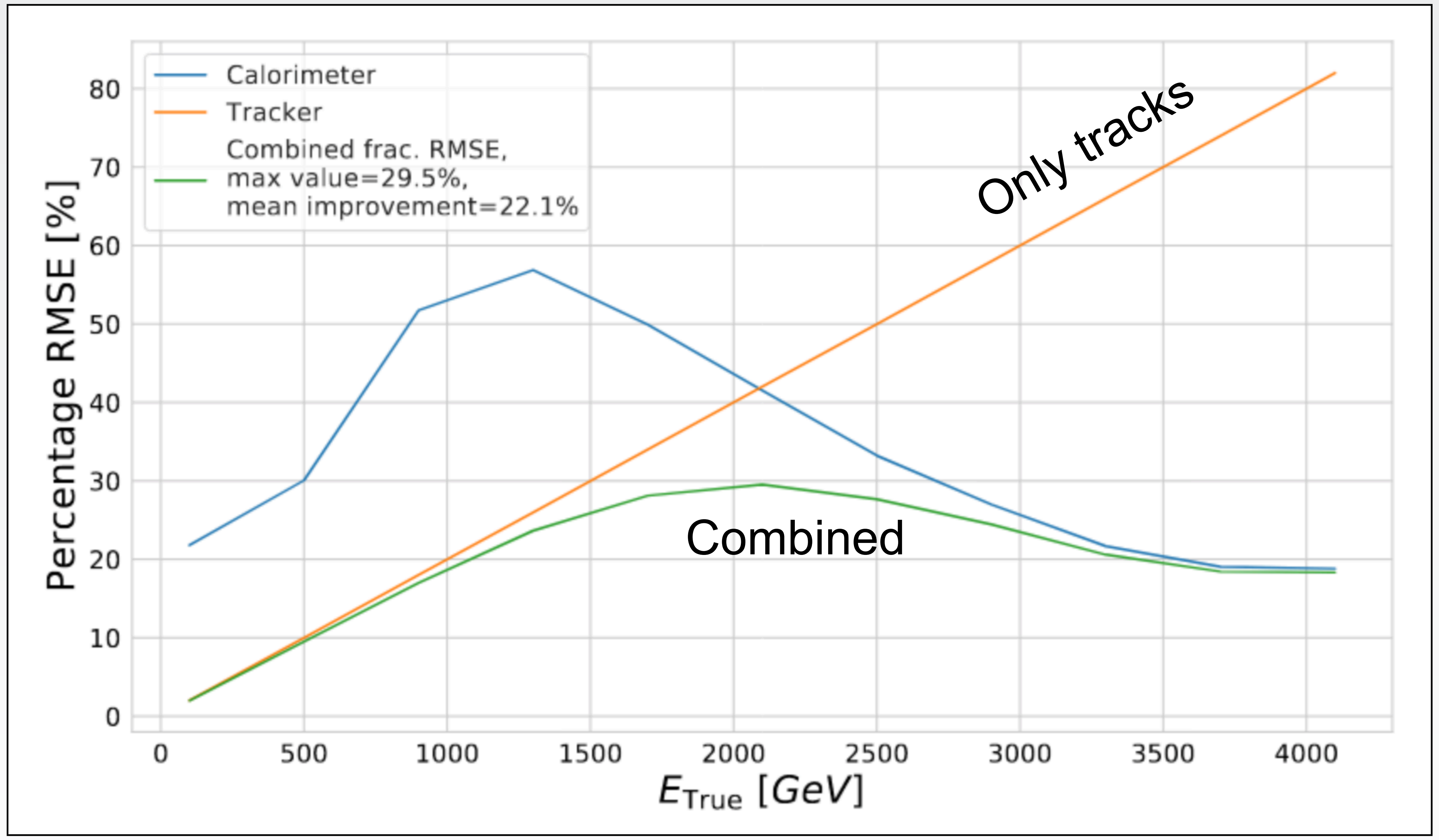


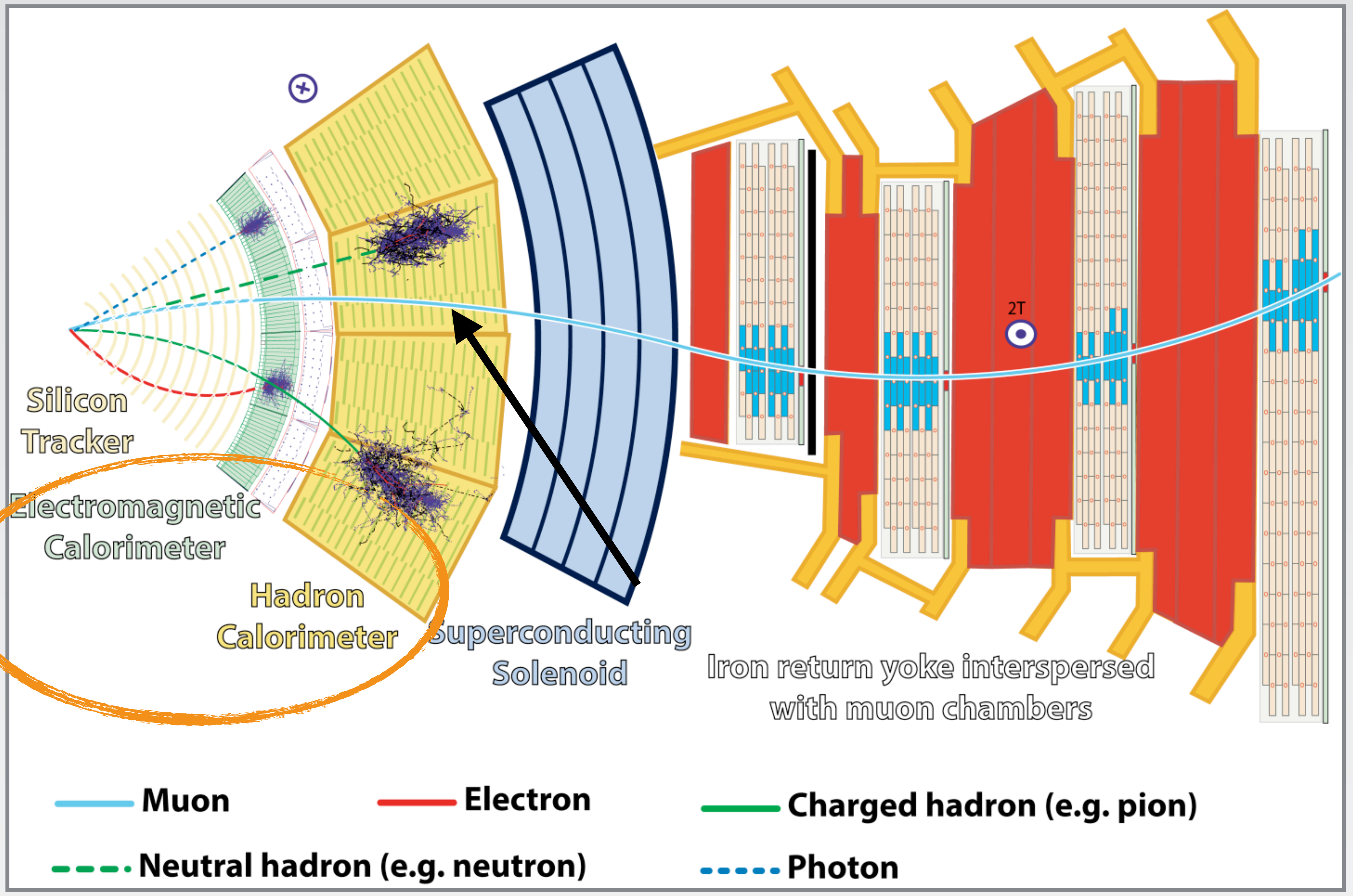
C. Neubüser, JK, P Lujan, arxiv:2101.08150, EPJC

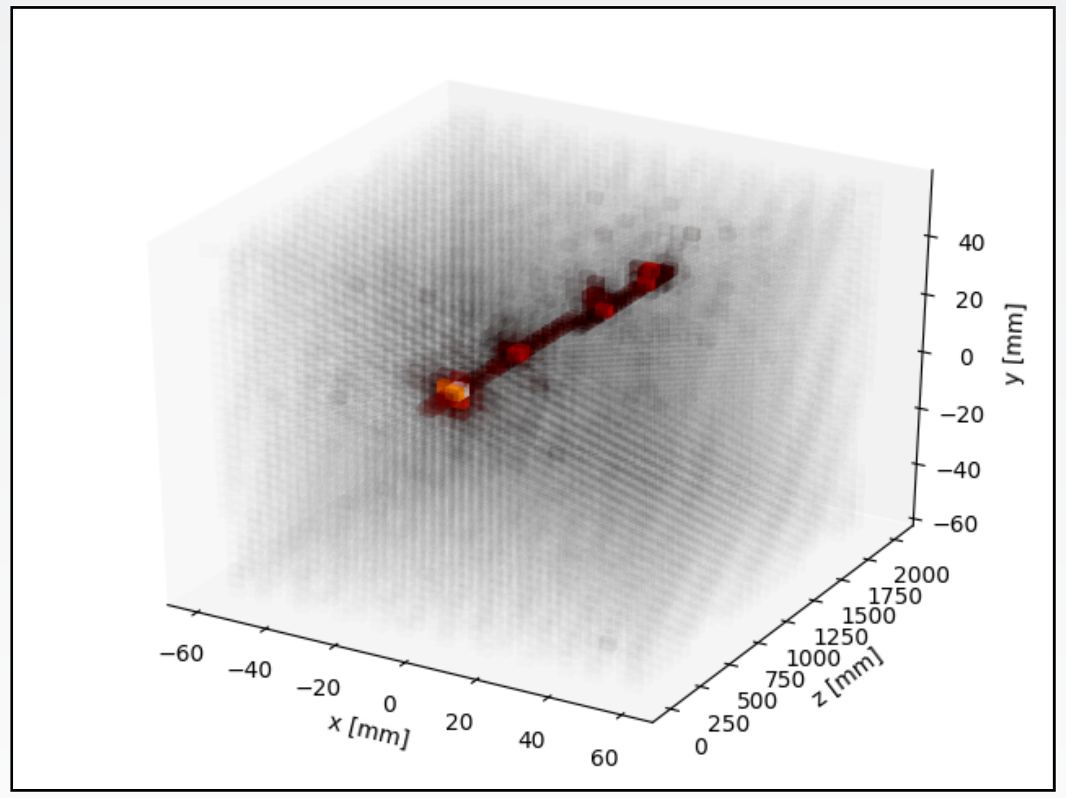
Use known sub detectors in a new way

- At future very high energy colliders
  - Muons will deposit more energy
  - Muons will bent less → tracks provide less information

- The pattern of radiation deposits contains information useful to regress the true muon energy, opens up new possibilities and impacts detector concepts
- Based on CNNs



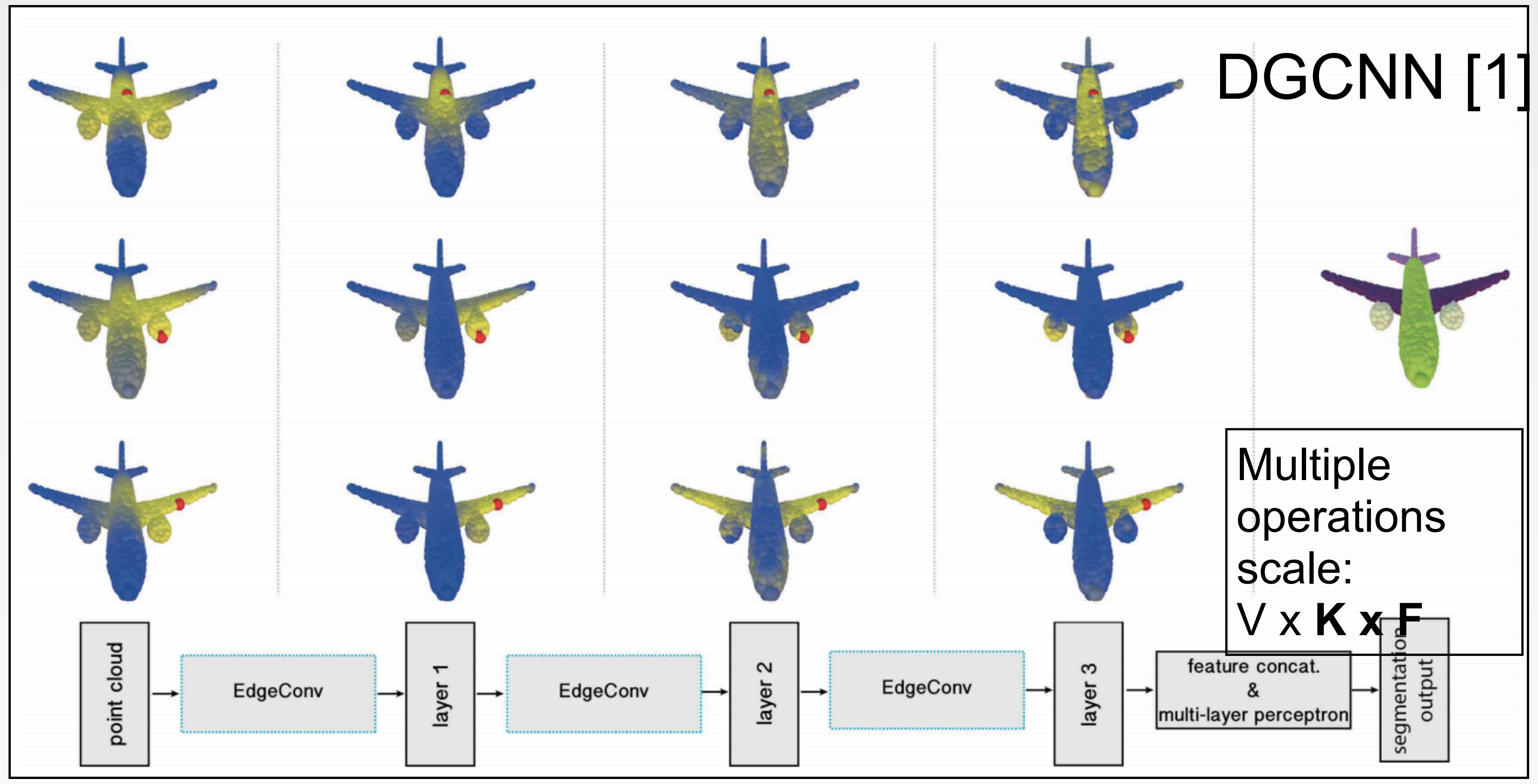




JK, G. Strong, et al., arXiv:2107.02119

Irregular Geometries

- Detectors are not grids of sensors
- The reconstruction needs to account for that
- Graph neural networks are a powerful solution
  - No sorting required
  - No grid
  - Sense of connection
  - Basic principle: information exchange through edges (connections)



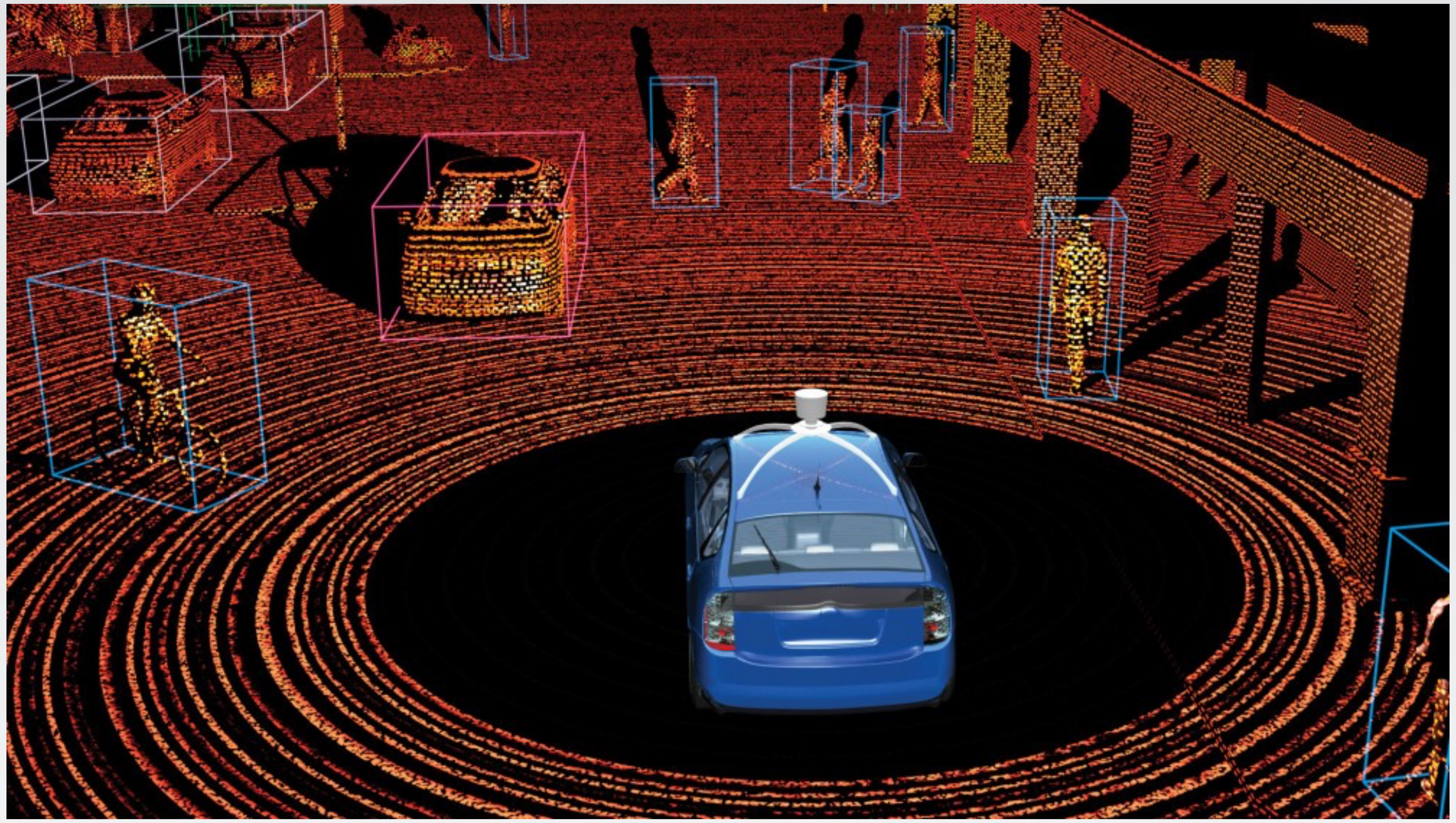
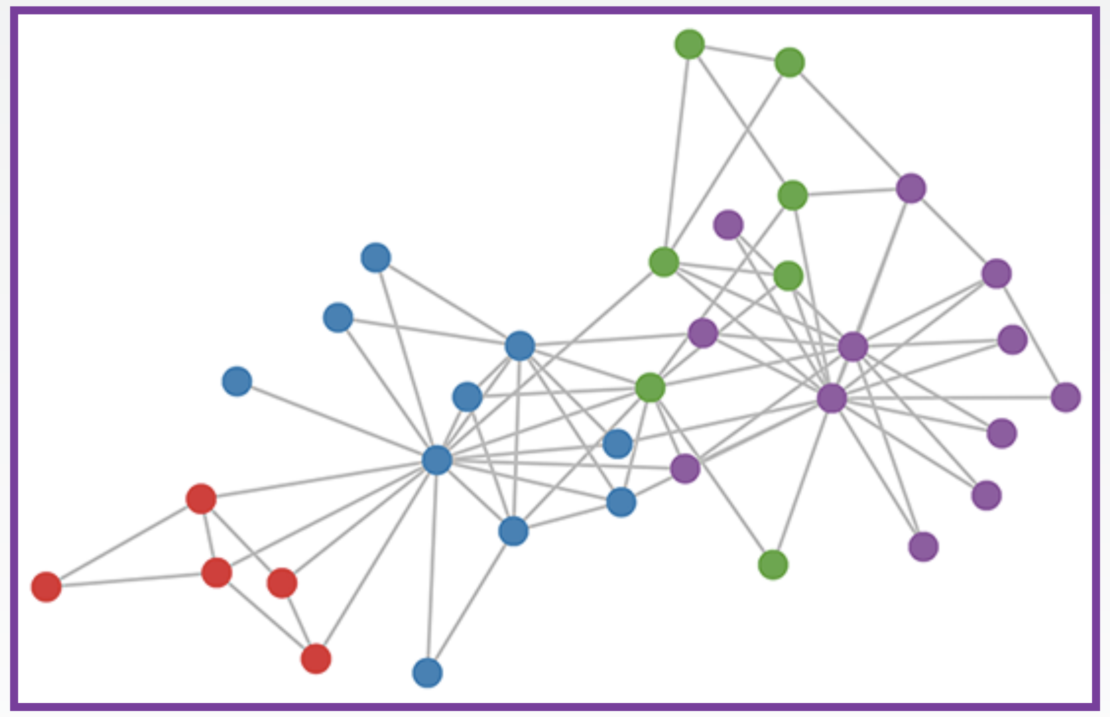


Image from https://news.voyage.auto/an-introduction-to-lidar-the-key-self-driving-car-sensor-a7e405590cff

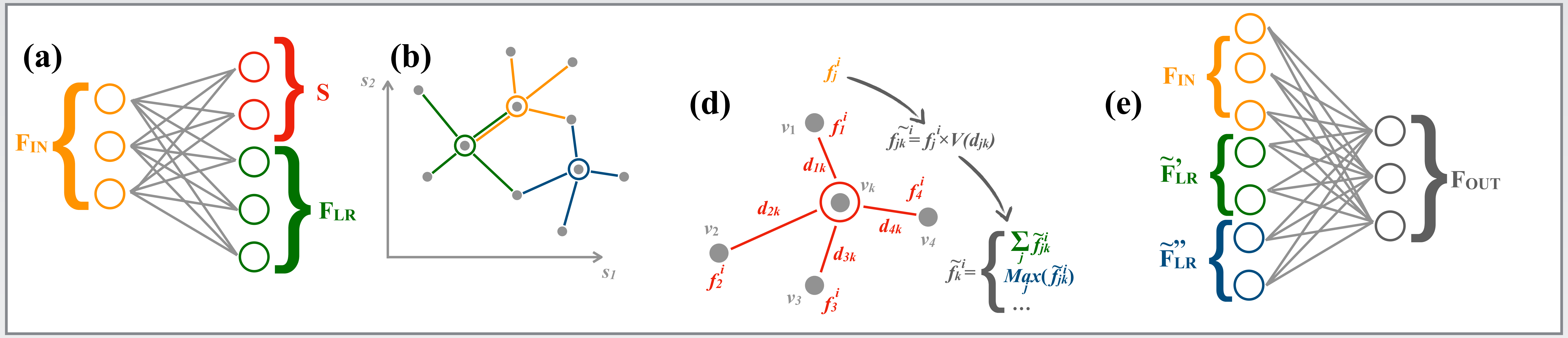


- A typical HEP detector has O(500k) active sensors each event
- The network needs to fit into the resources

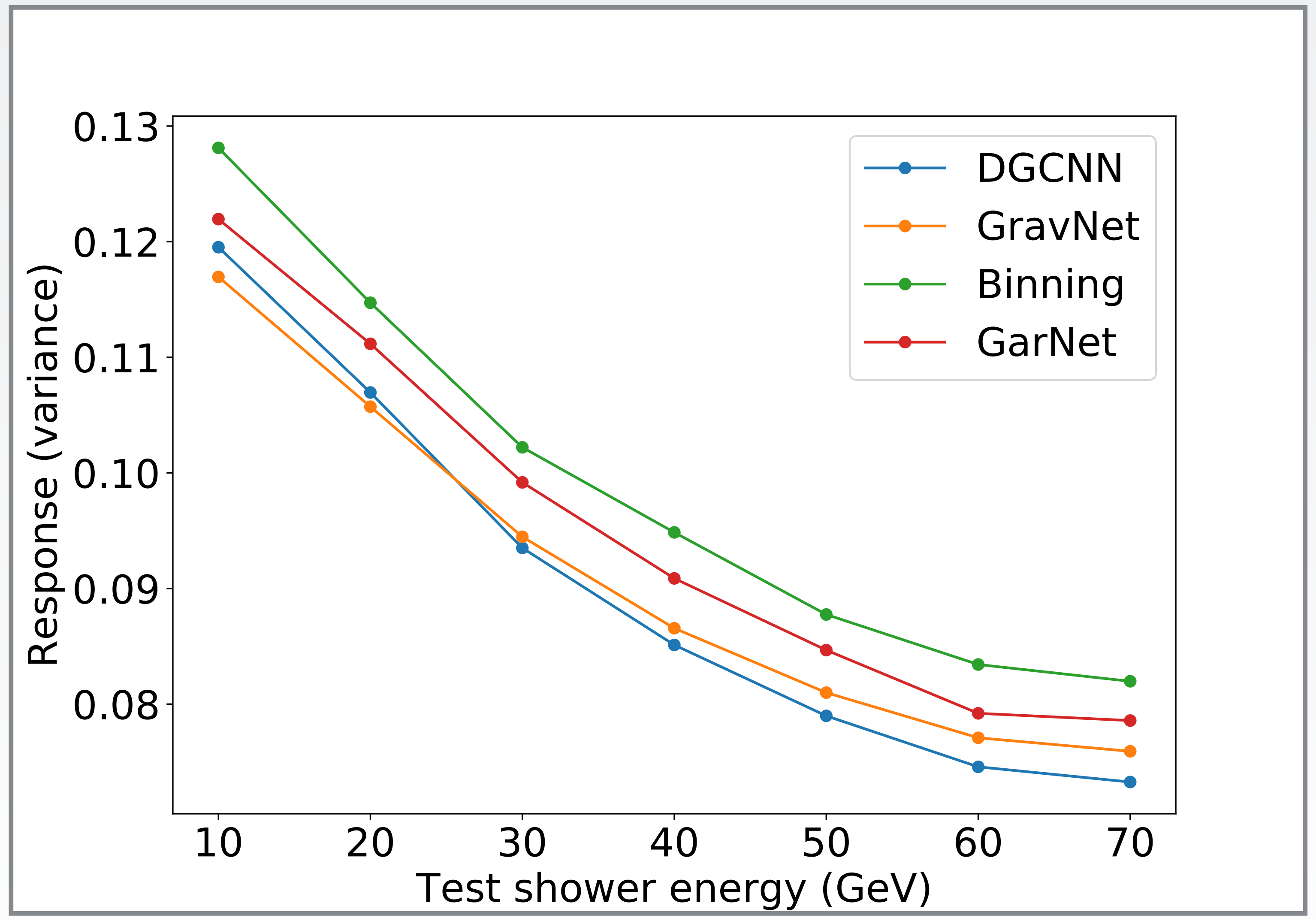
[1] Y. Wang, et al, arXiv:1801.07829

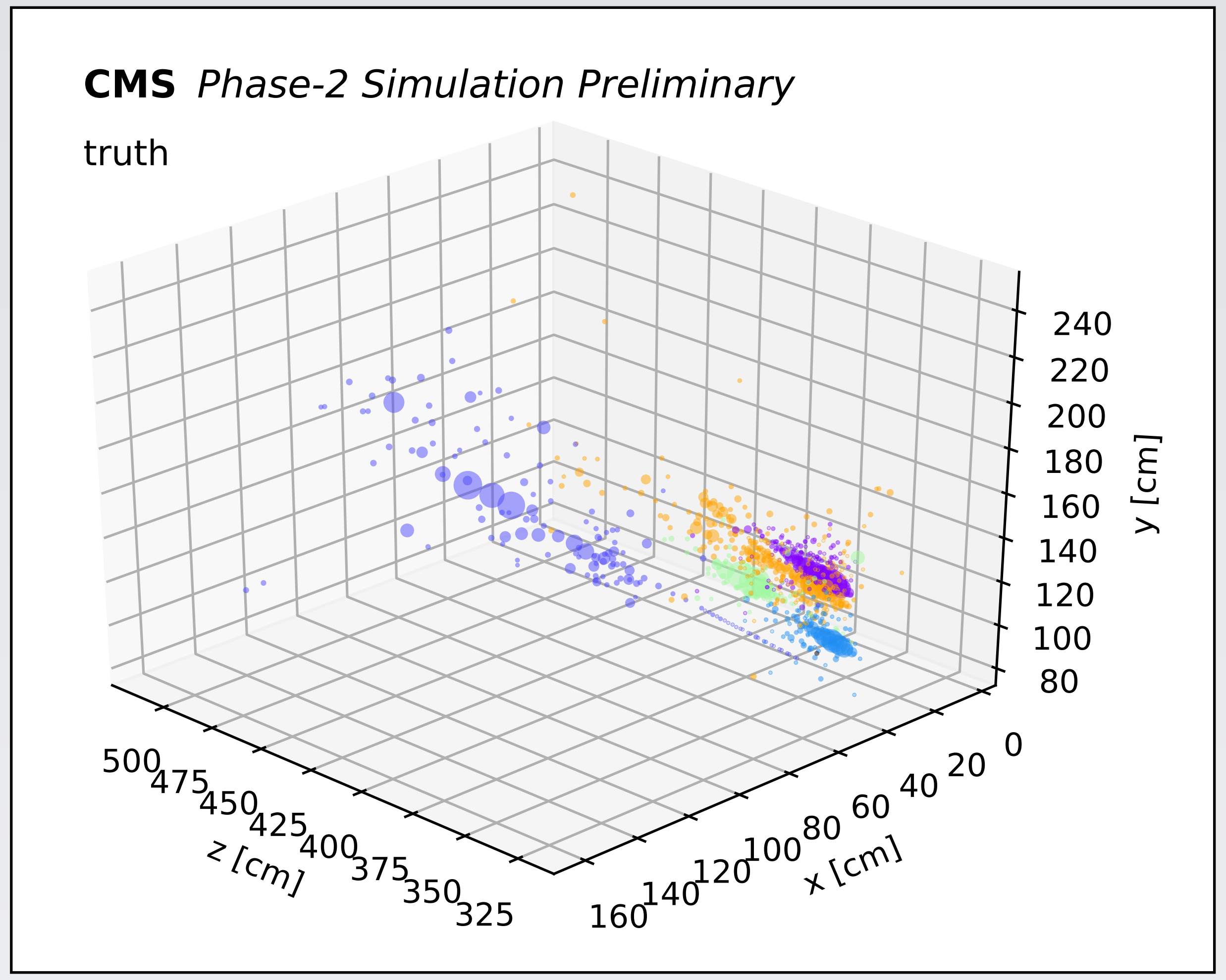
GravNet

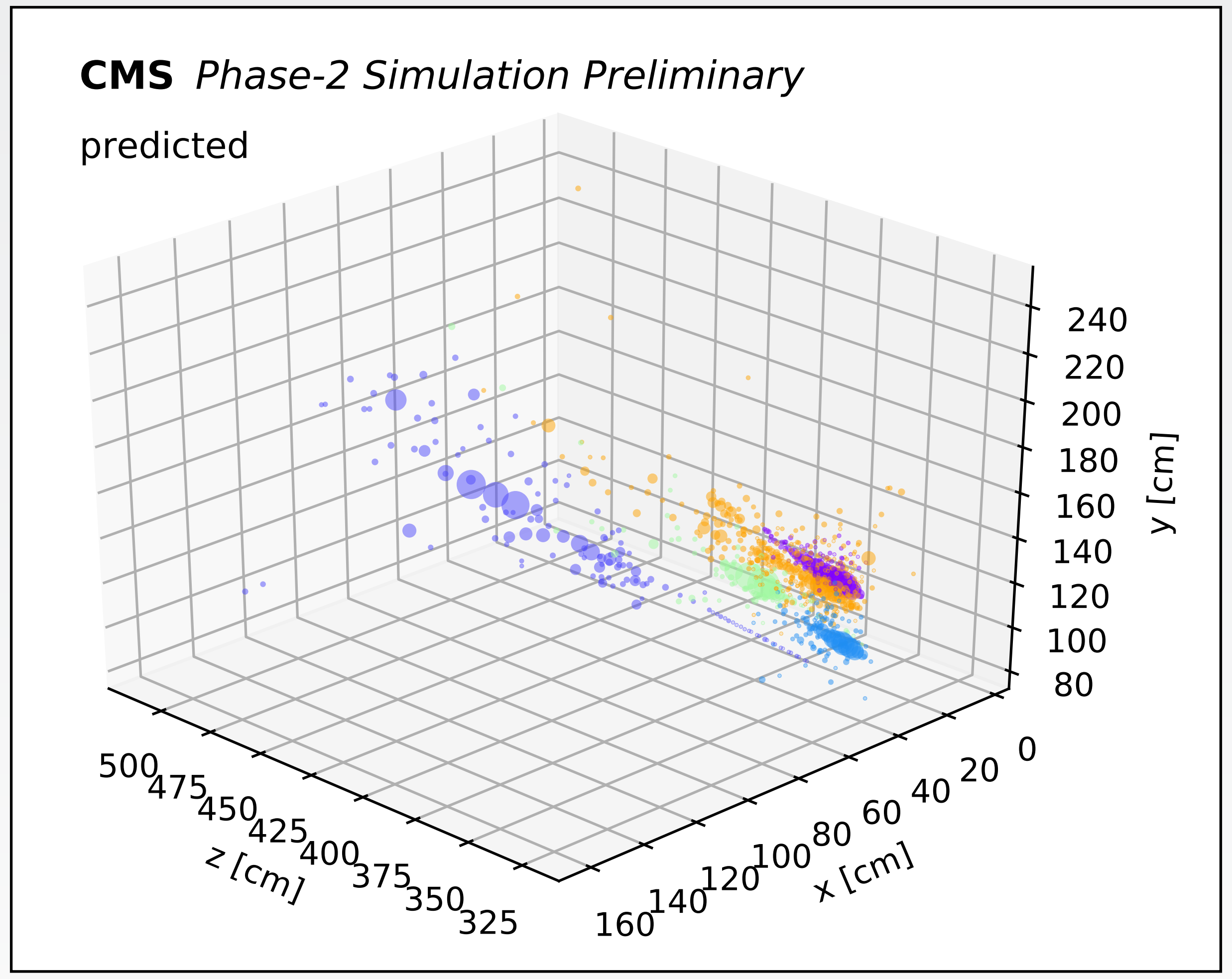
- Developed to overcome resource limitation
- Main 'trick': split into low dimensional coordinate and high dimensional feature space



- Tested on a HEP calorimeter reconstruction task
- Up to 2 orders of magnitude improvement w.r.t. resources: ~500k hits can be processed







GravNet in torch_geometric!

https://pytorch-geometric.readthedocs.io/en/latest/modules/nn.html#torch_geometric.nn.conv.GravNetConv

Fused kernels

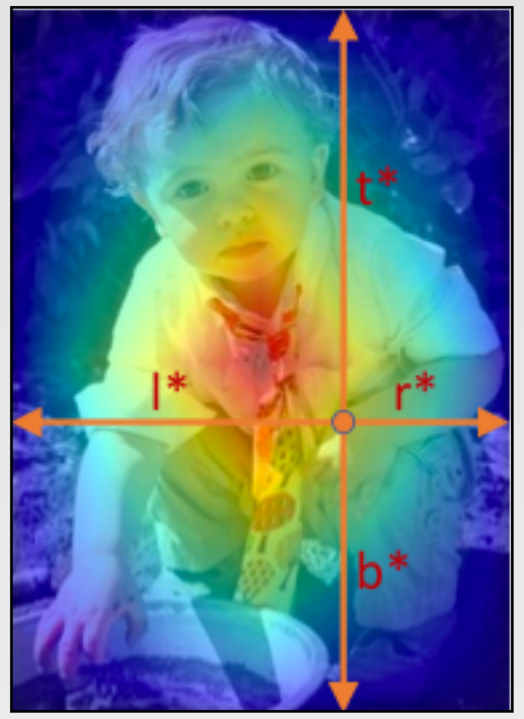
https://github.com/cms-pepr/pytorch_cmspepr

S.R. Qasim, J. K, Y. Iiyama, M Pierini,
arXiv:1902.07987
CMS DP-2020/001

Multi-particle reconstruction

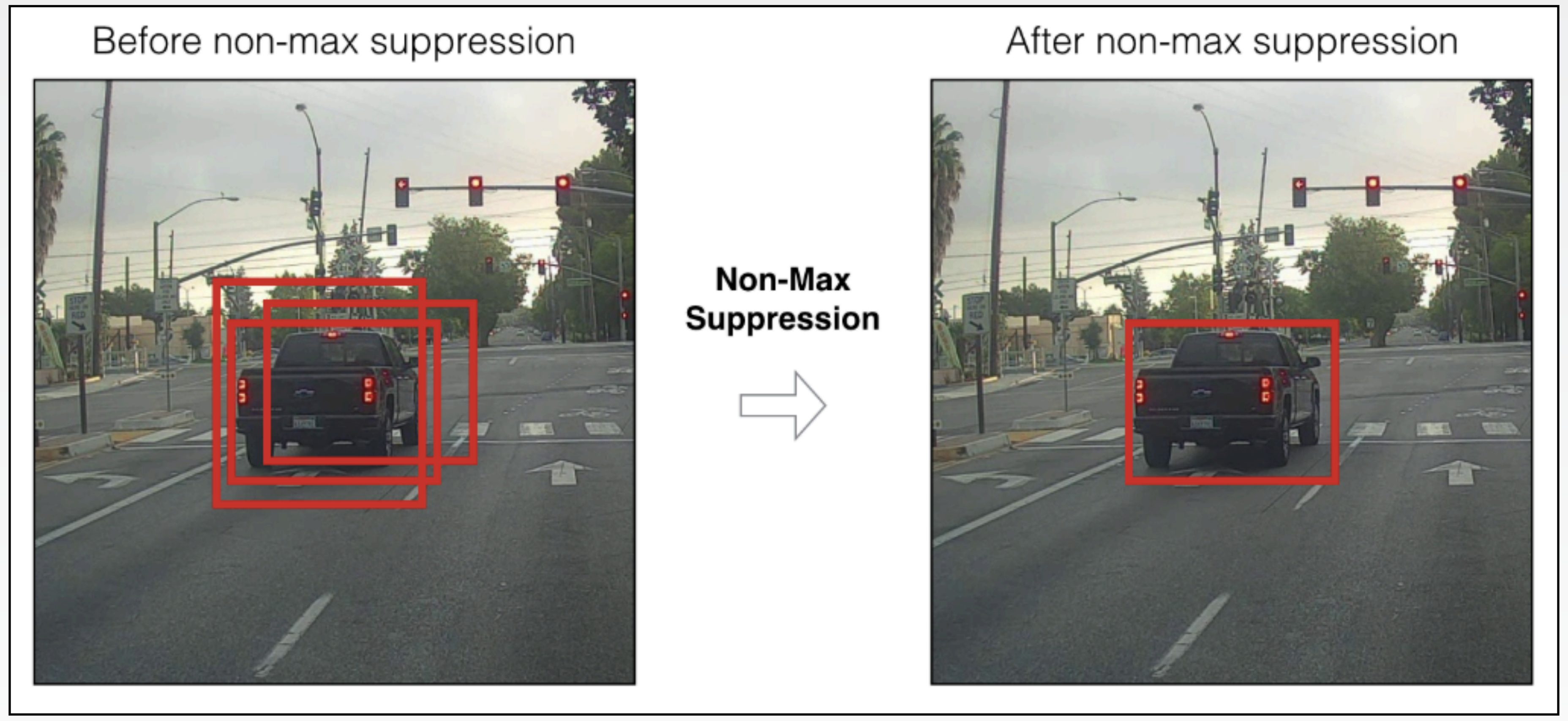
The usual chain

- Local seeding (pattern recognition)
- Local clustering (pattern recognition)
- Software compensation (pattern recognition)
- Identification (pattern recognition)
- Linking of individual detector parts (pattern recognition)



Challenges

- A priori unknown number of particles to reconstruct
- Particles are not dense objects with clean centres and boundaries
- The input data is represented by point clouds



N. Wang et al, arXiv:1904.01355
X. Zhou et al, arXiv:1904.07850

- Maximum number of objects per image/point cloud: number of pixels/vertices

- Learn to move pixels towards the object center
- Map to Gaussian probability

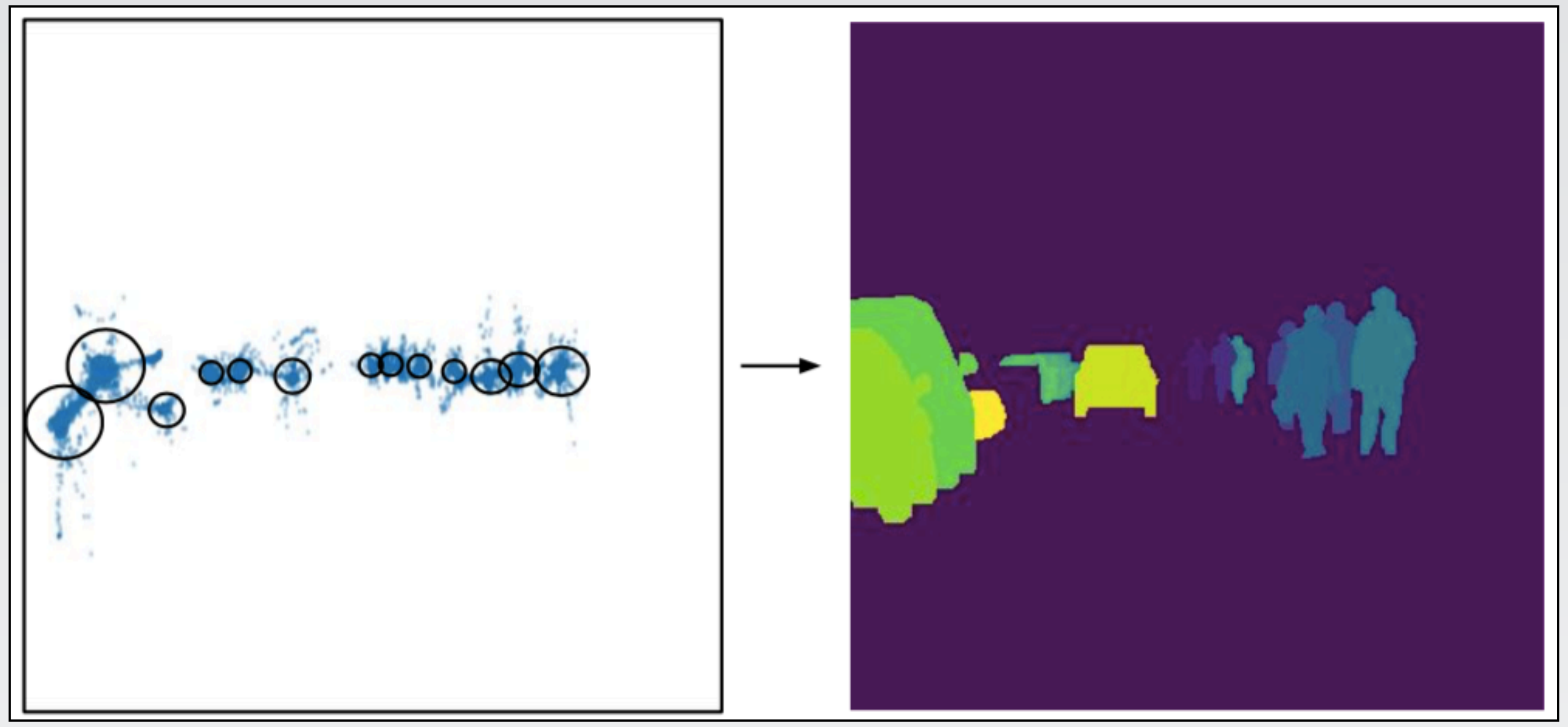
$$\phi_k(e_i) = \exp\left(-\frac{\|e_i - C_k\|^2}{2\sigma_k^2}\right)$$

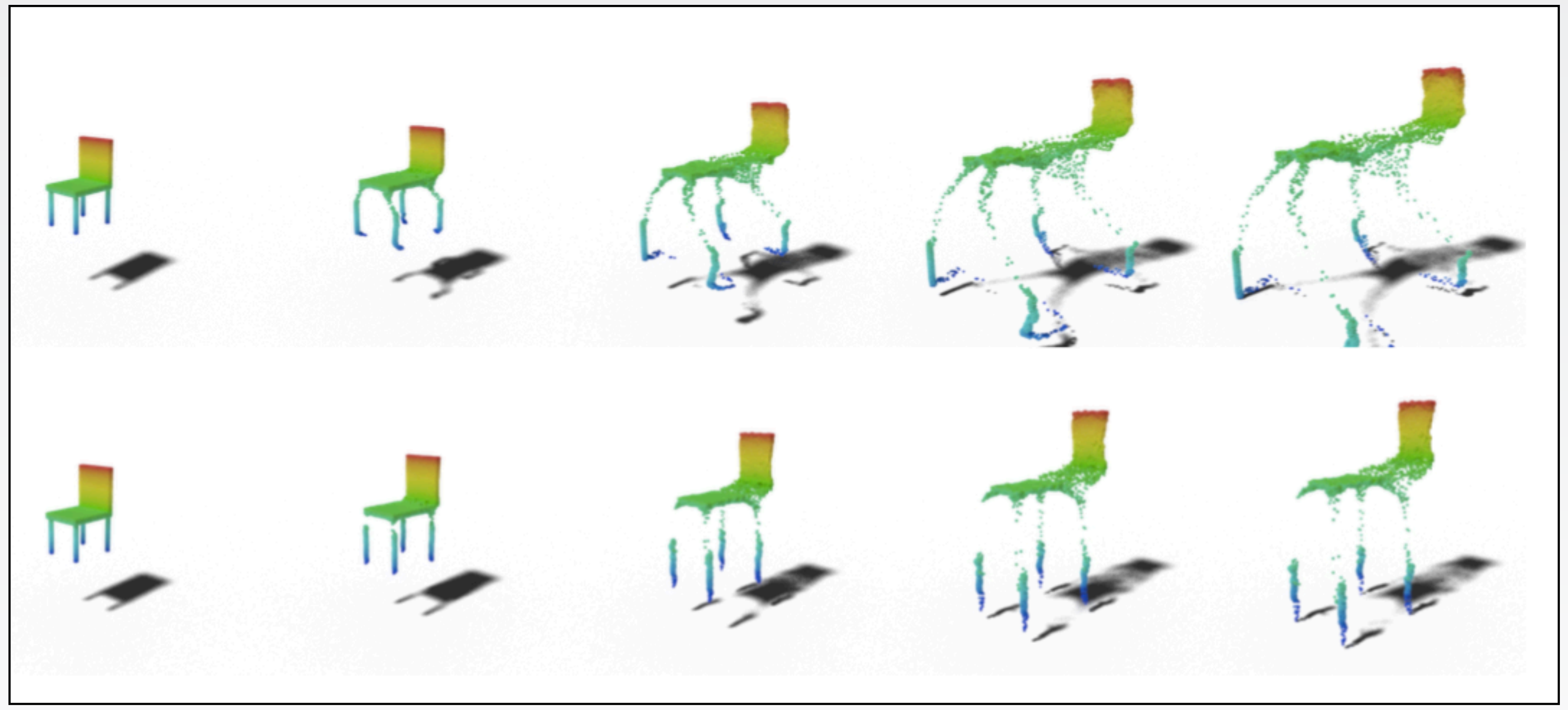
- Assign seed score

$$\mathcal{L}_{\text{seed}} = \frac{1}{\mathrm{N}} \sum_{i}^{\mathrm{N}} \mathbb{1}_{\{s_i \in S_k\}} \|s_i - \phi_k(e_i)\|^2 + \mathbb{1}_{\{s_i \in \text{bg}\}} \|s_i - 0\|^2$$

- Collect (from highest seeds score) around the seeds

- *'Only' performs segmentation*
- *Heavily relies on the center of an object*
  - *Problematic concept for particles*





D. Neven et al, arXiv:1906.11109
B. Zhang, P. Wonka, arXiv:1912.00145

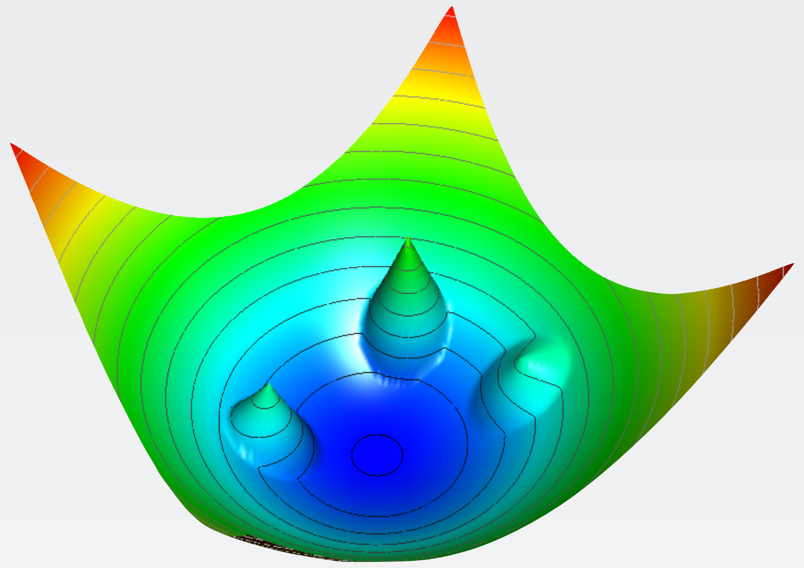
Object Condensation

- Merge object property determination and segmentation
- Create a decoupled ‘clustering’ space
  - Created by potentials
- Assign ‘condensation score’ → charge
  - Highest score condensation points carry object properties
- Push non-differentiable ‘clustering’ step towards the very end

- Segmentation

$$\breve{V}_k(x) = ||x - x_\alpha||^2 q_{\alpha k}, \text{ and}$$

$$\hat{V}_k(x) = \max(0, 1 - ||x - x_\alpha||) q_{\alpha k}.$$



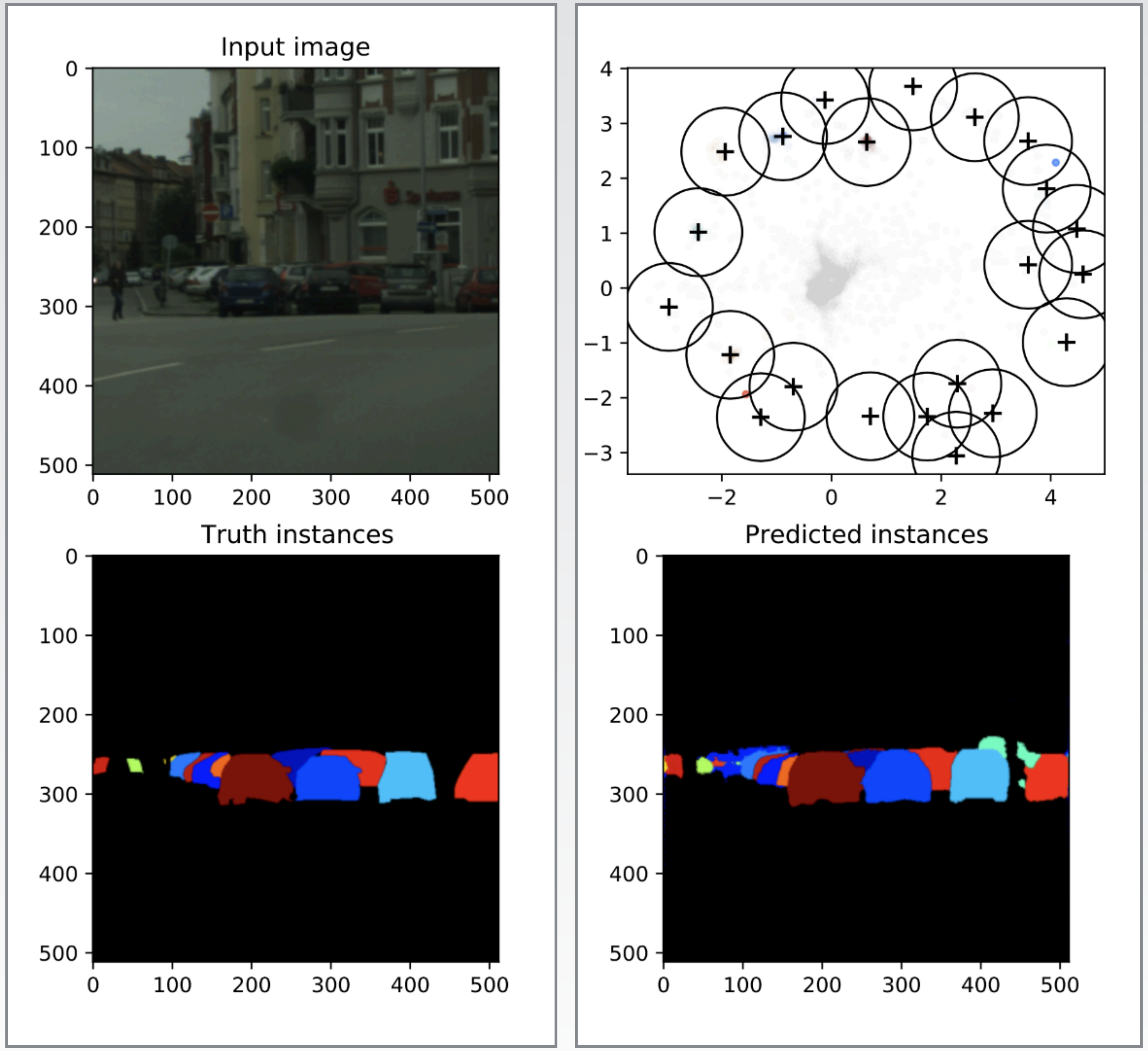
- Reconstruction efficiency and noise

$$L_\beta = \frac{1}{K}\sum_k (1-\beta_{\alpha k}) + s_B \frac{1}{N_B}\sum_i^N n_i \beta_i,$$

- Object properties

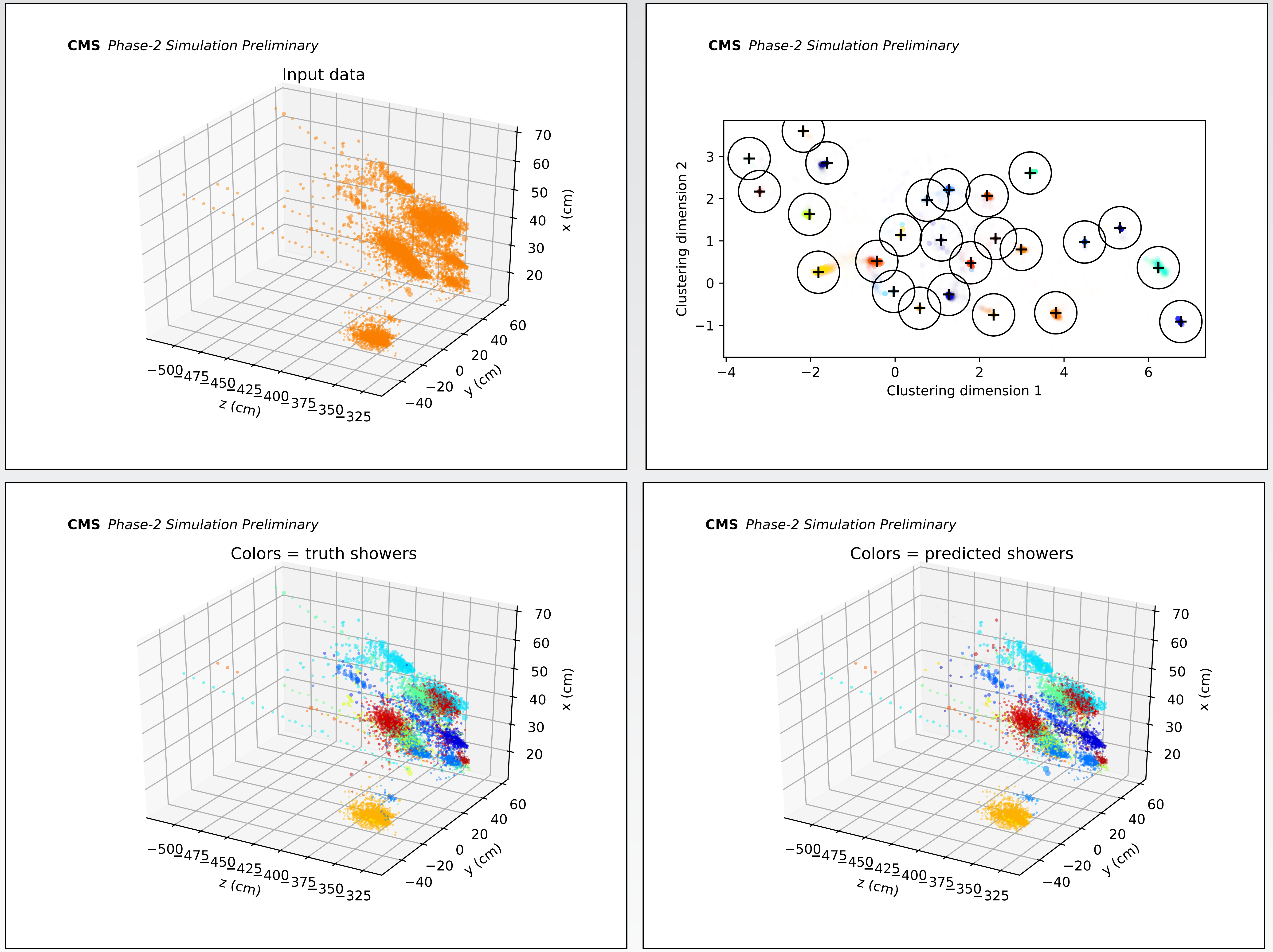
$$L_p = \frac{1}{\sum_{i=0}^N (1-n_i)\,\mathrm{arctanh}^2\,\beta_i}\sum_{i=0}^N L(t_i, p_i)(1-n_i)\,\mathrm{arctanh}^2\,\beta_i$$

➡Generalises to image data

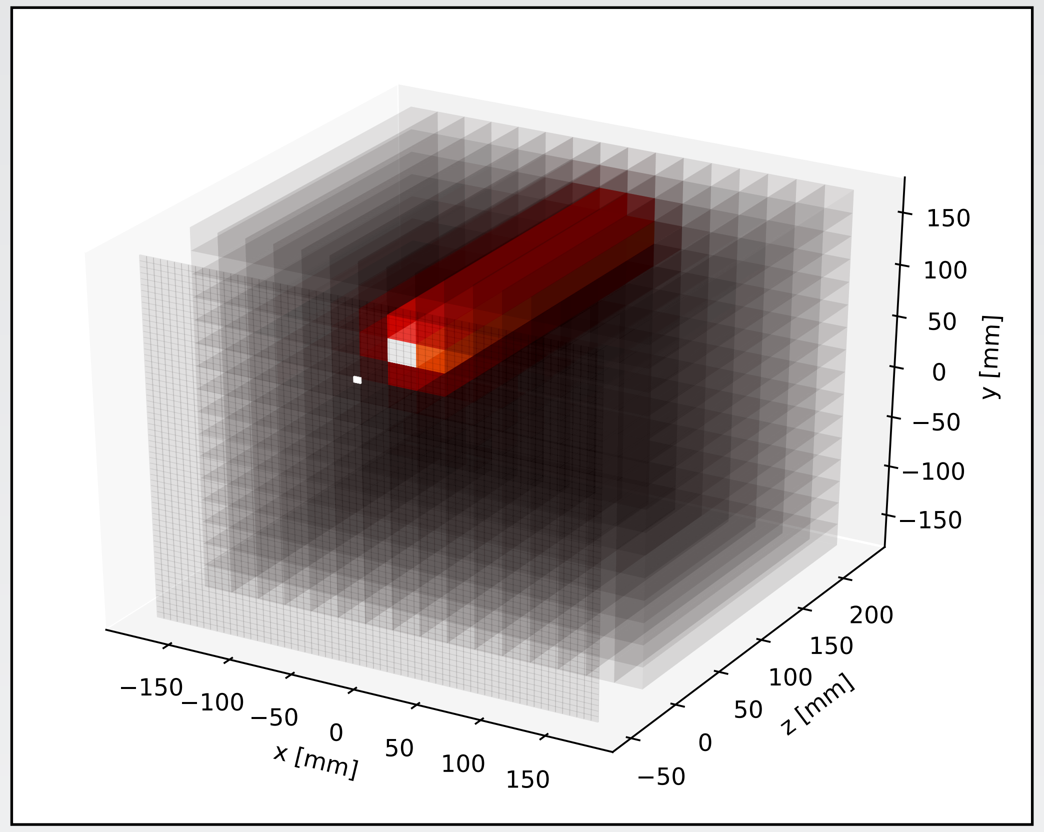


JK, arxiv:2002.03605, EPJC

High granular calorimeter application



- Differentiable one-shot reconstruction from hits to final state particles

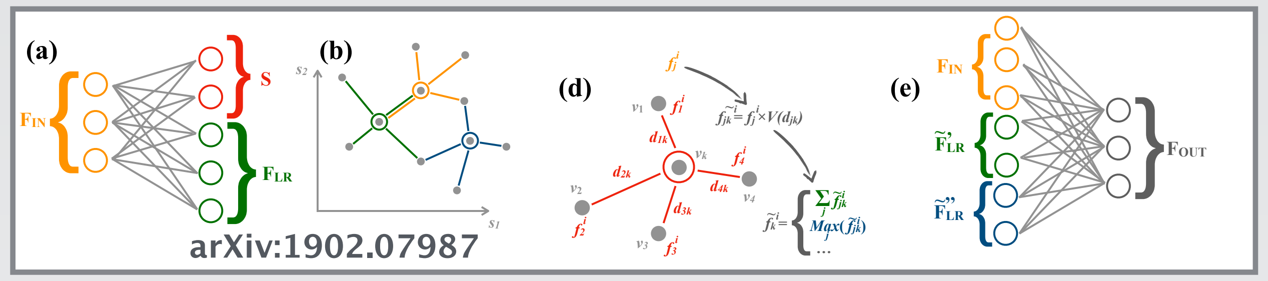


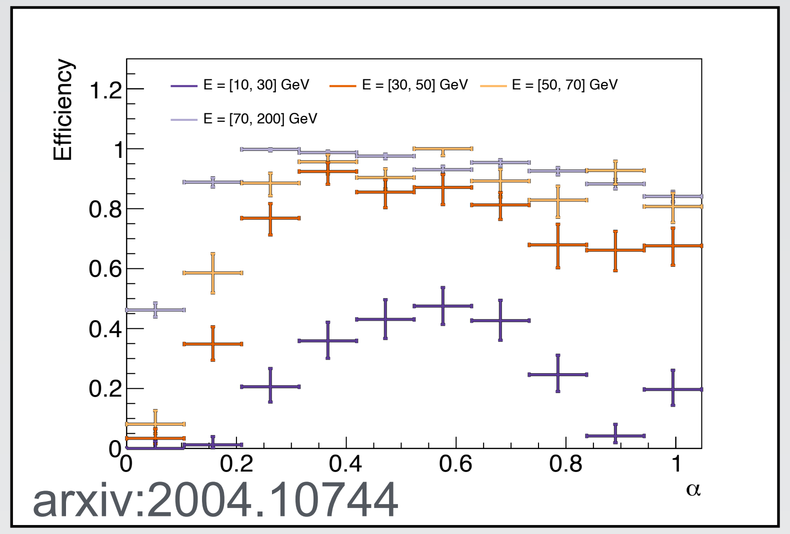
- Can also be applied to information from different sub detectors

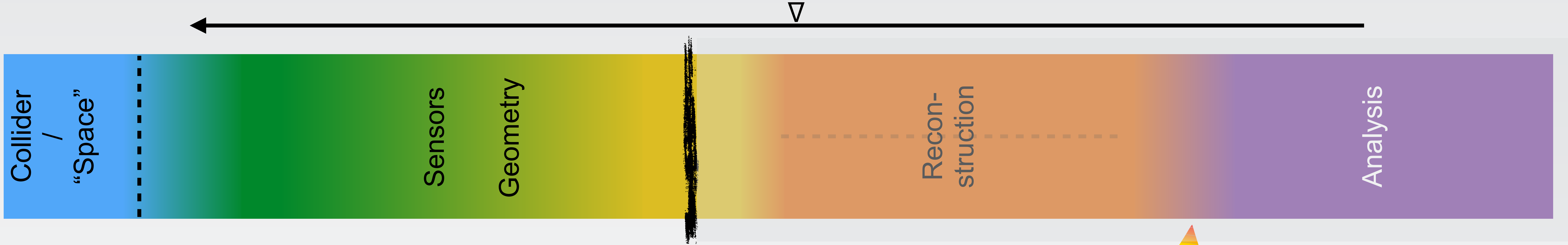
The usual chain

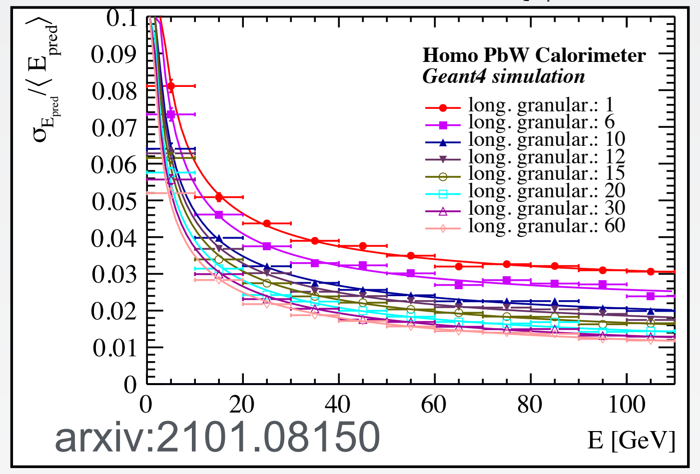
✓Local seeding (pattern recognition)
✓Local clustering (pattern recognition)
✓Software compensation (pattern recognition)
✓Identification (pattern recognition)
✓Linking of individual detector parts (pattern recognition)

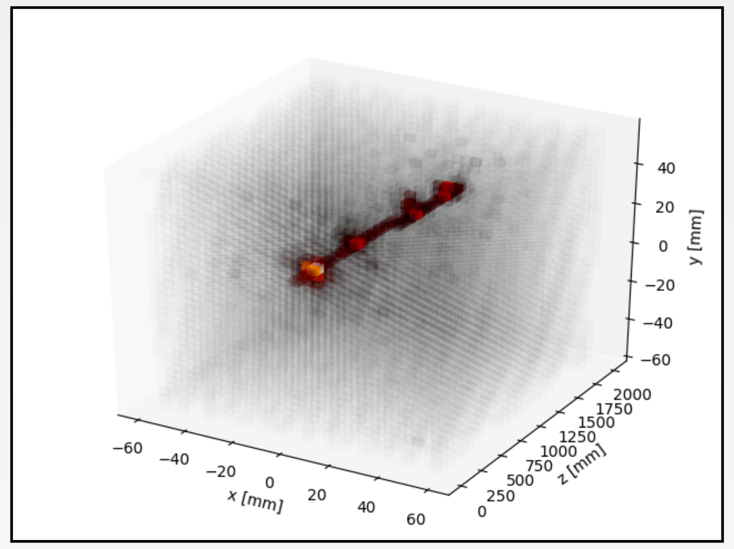
What do we already have

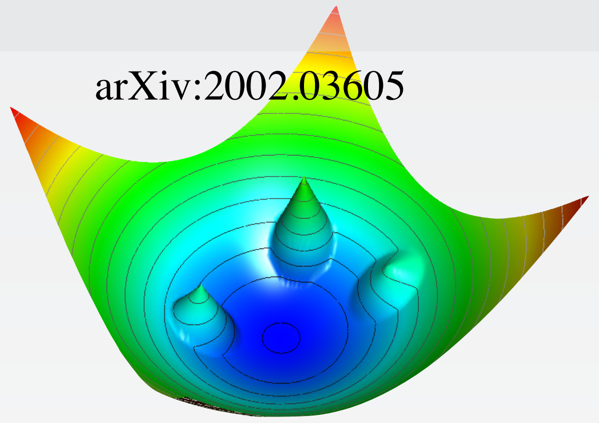

arXiv:1902.07987

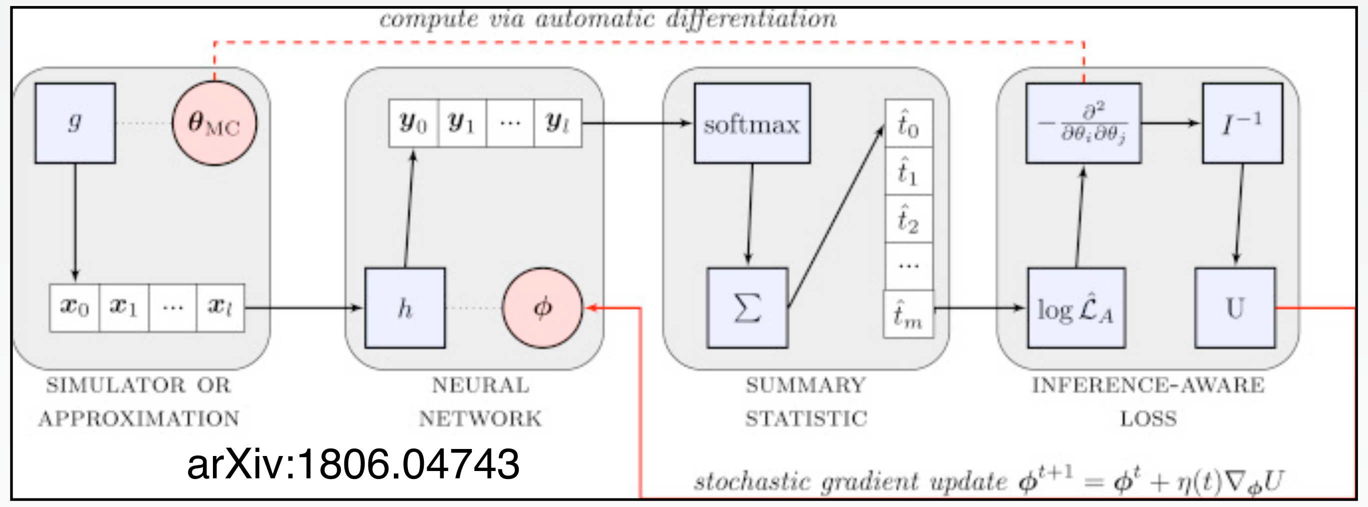

arxiv:2004.10744

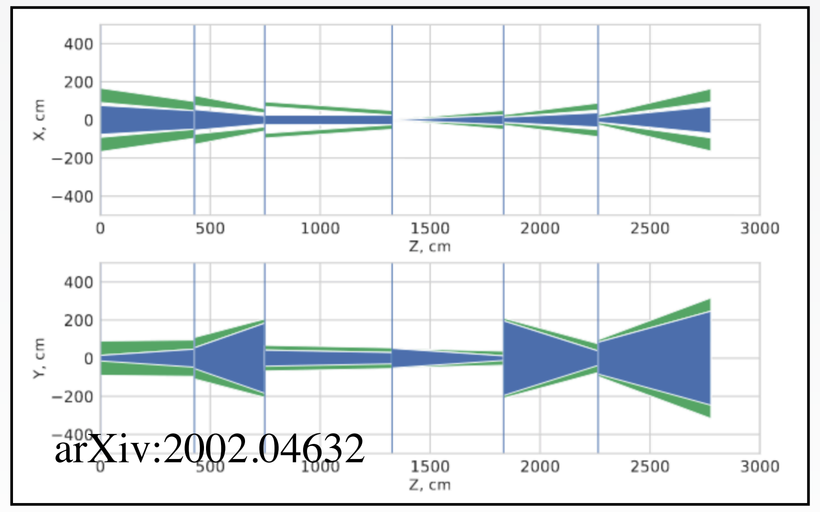



arxiv:2101.08150

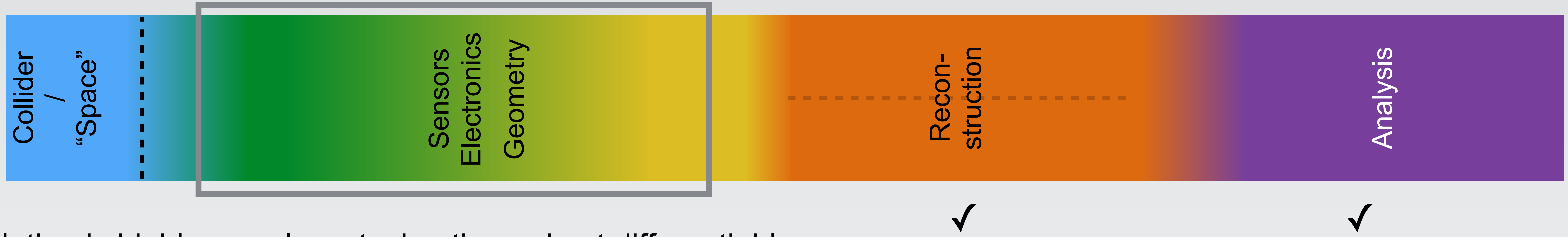



arXiv:2002.03605

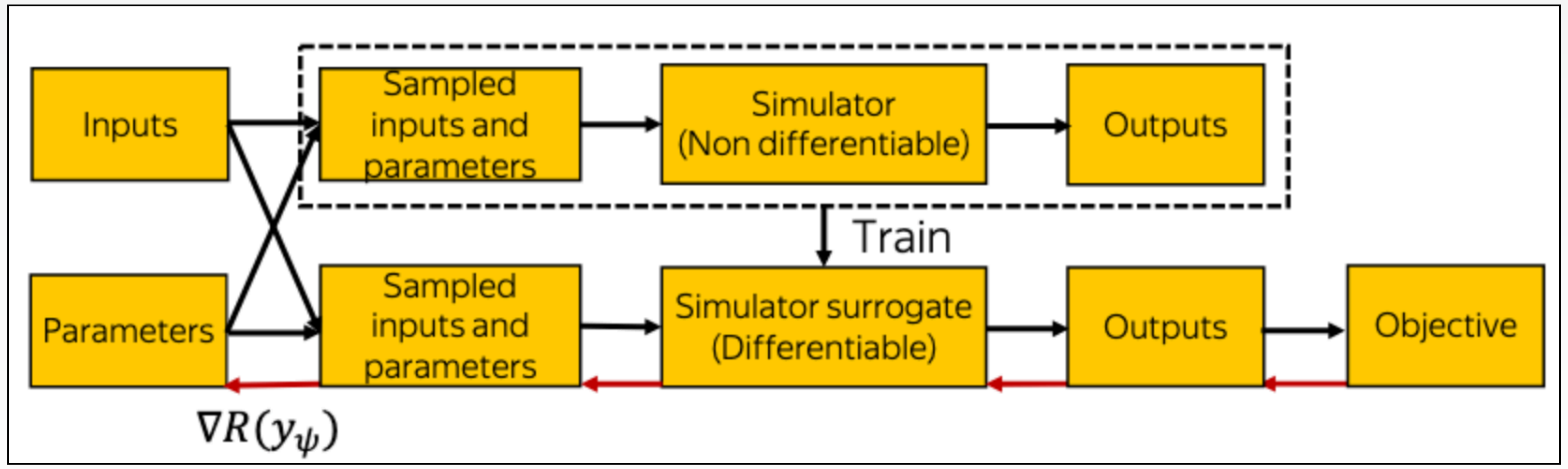

arXiv:1806.04743

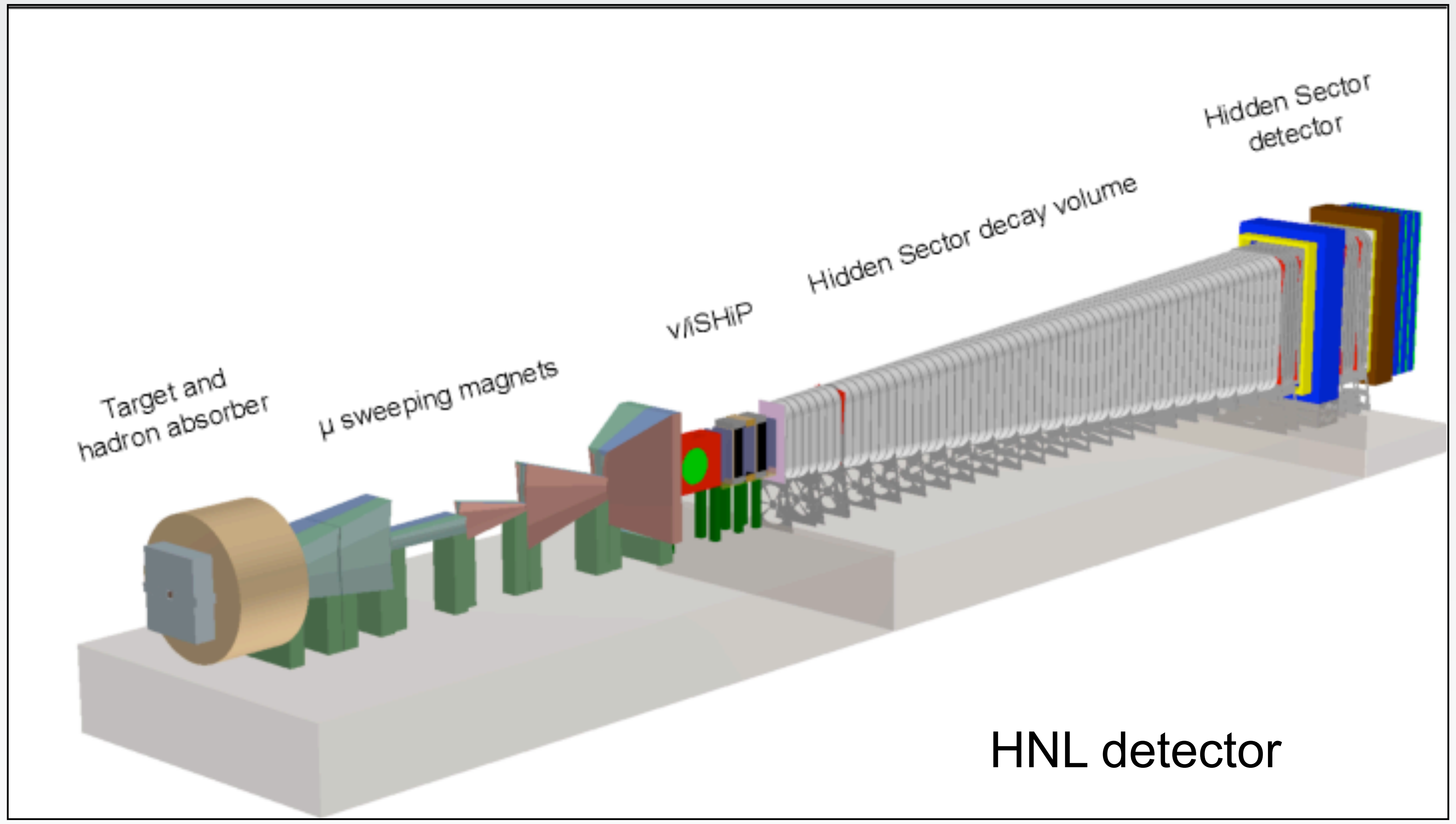

arXiv:2002.04632

Simulation



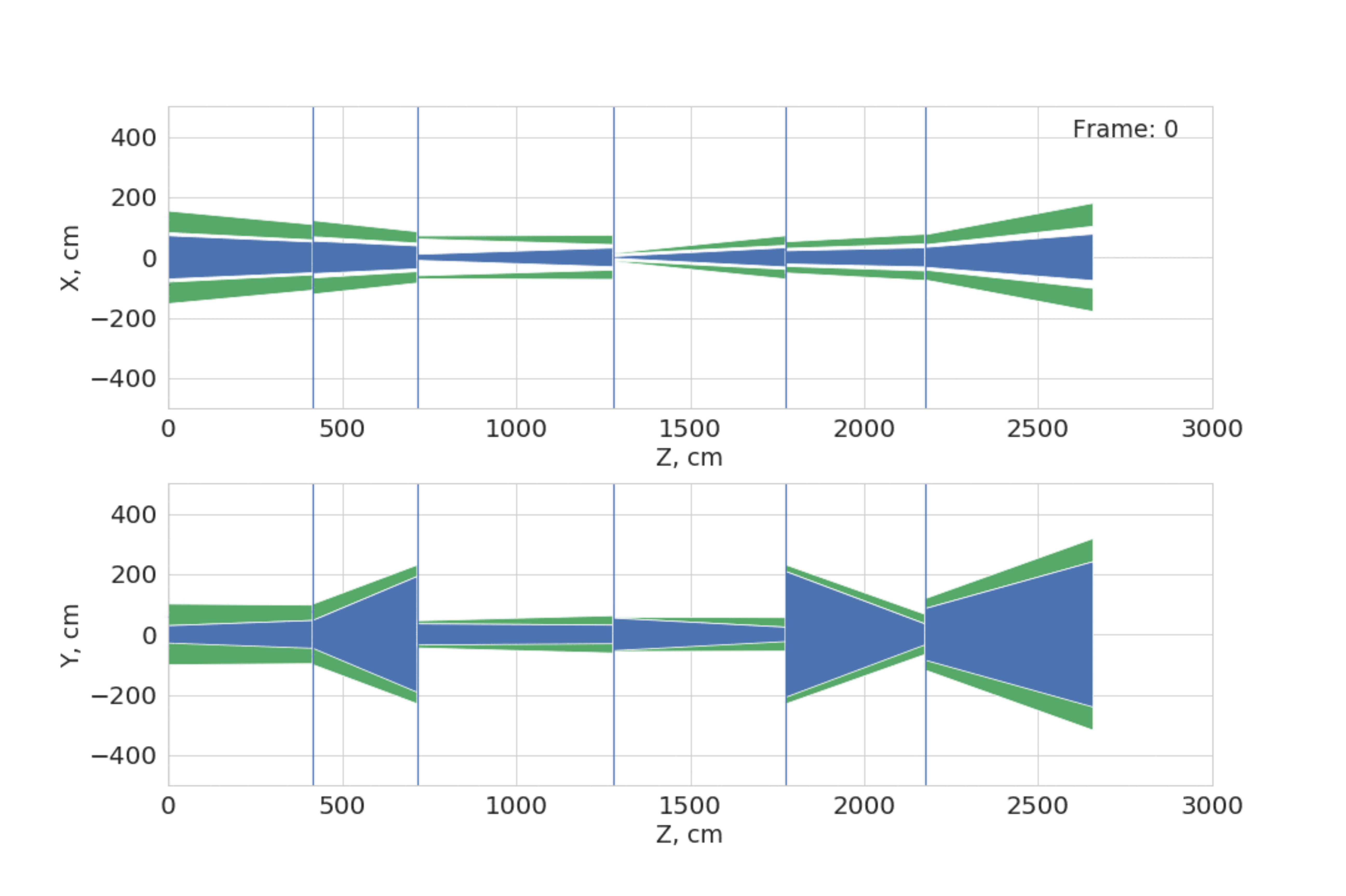
- Our simulation is highly complex, stochastic, and not differentiable
- Some parameters inherently have no gradient: e.g. adding/removing a sensor layer, switching positions, …
  - There are ideas, and some developments in the direction of solving this
  - This is a very interesting conceptual challenge to contribute to!
- Example: use **local surrogates of the gradient (GAN)** for optimising the SHIP muon shielding

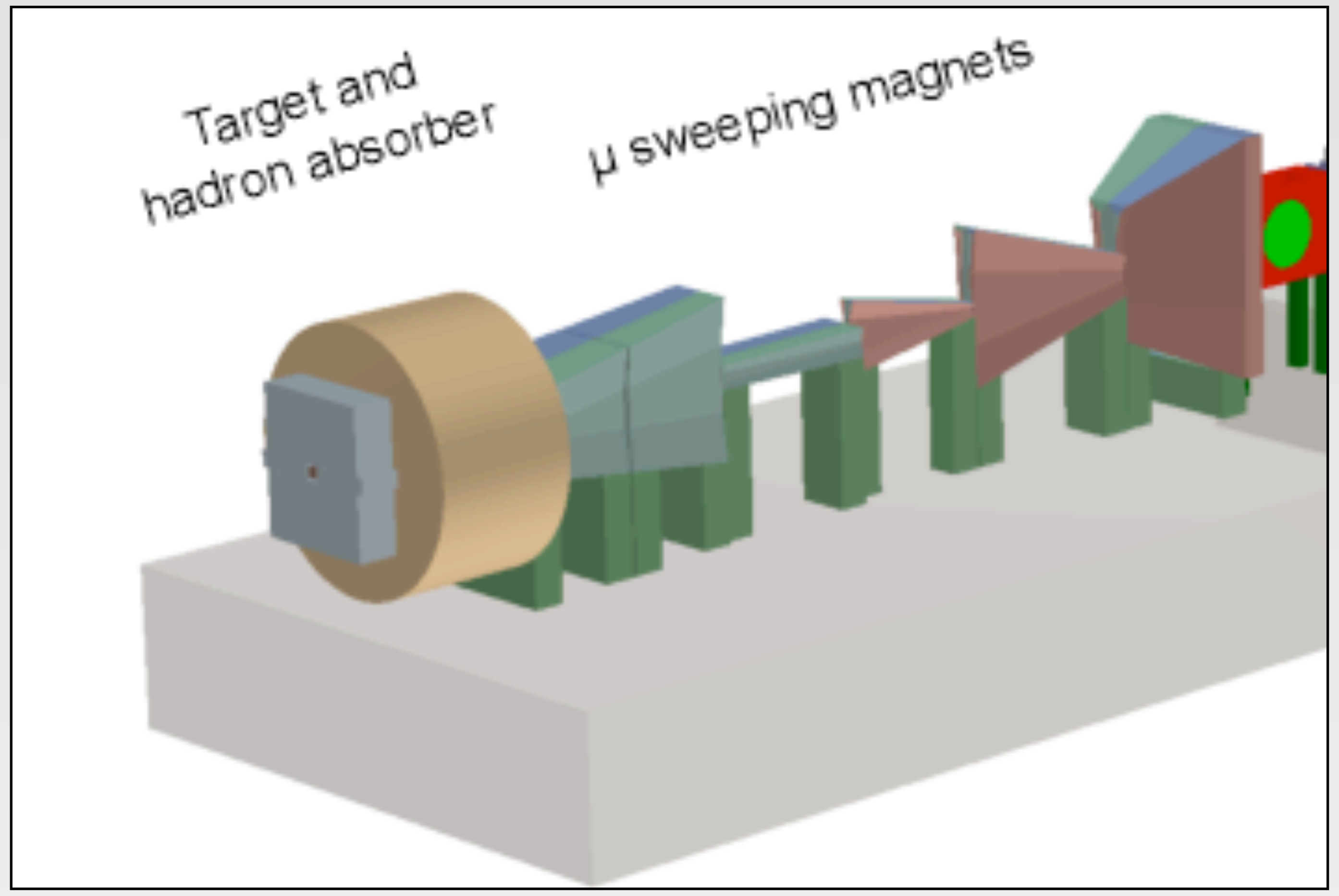




S. Shirobokov, A. Ustyuzhanin, A. Güneş Badyin et al., arXiv:2002.04632

Sweeping magnet optimisation





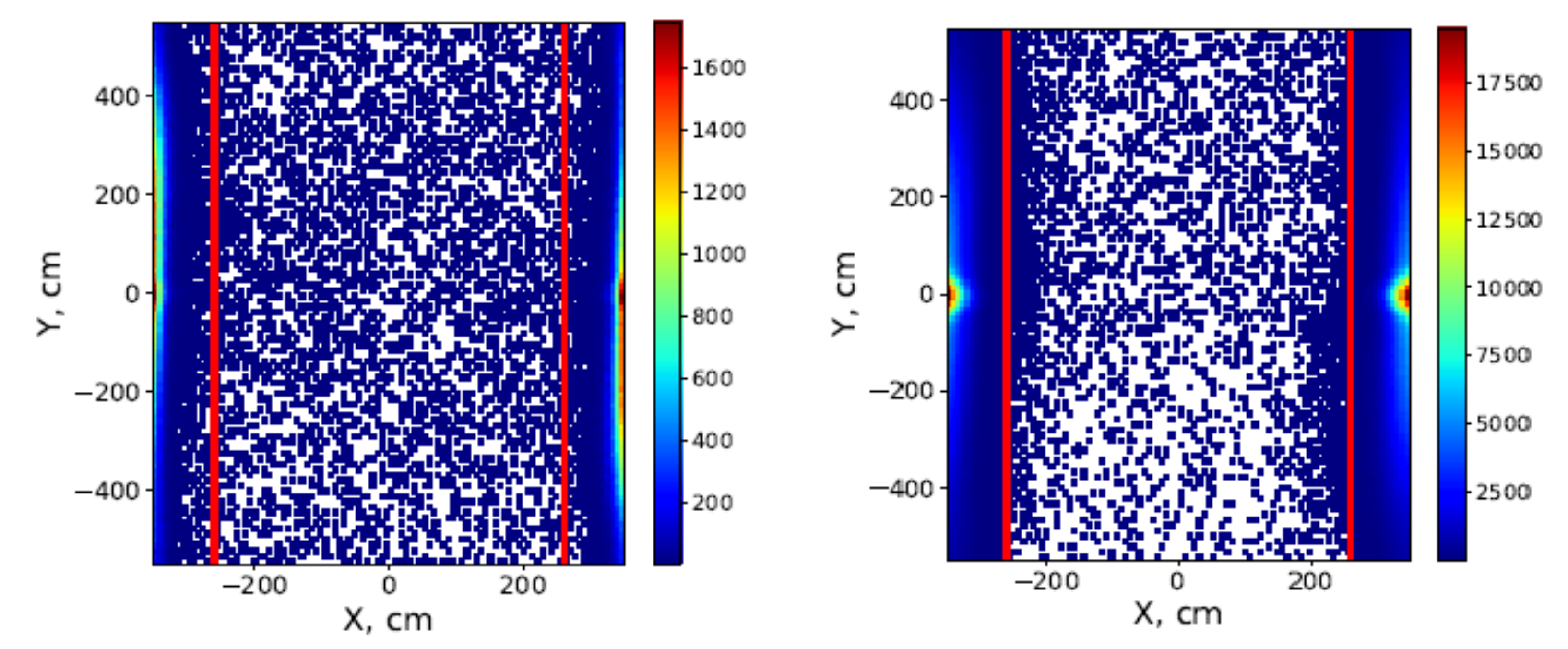


Figure 7. Muon hits distribution in the detection apparatus (depicted as red contour) obtained by Bayesian optimization (Left) and by L-GSO (Right), showing better distribution. Color represents number of the hits in a bin.

- Local differentiable surrogates can help solve the problem of non-differentiable simulation

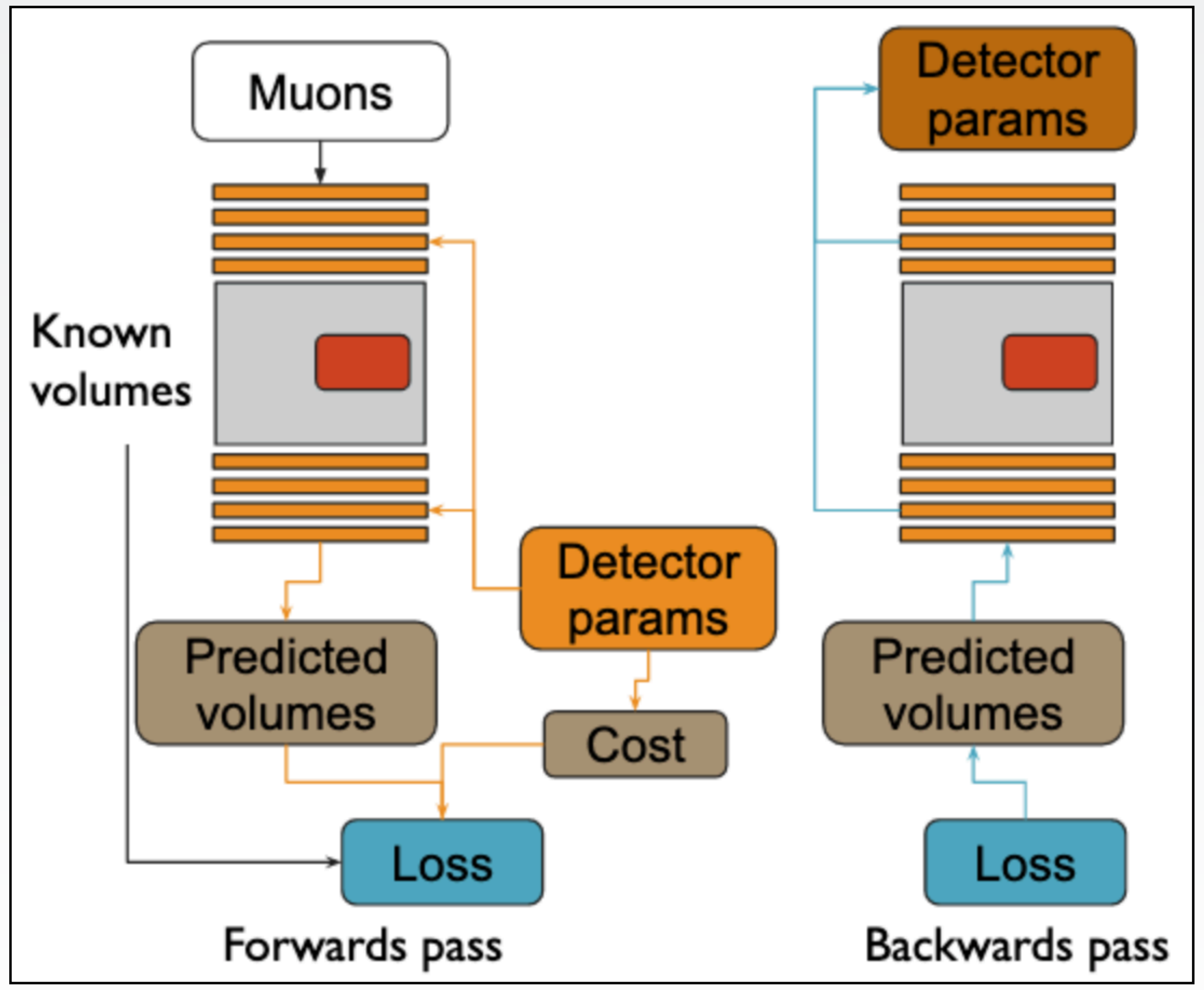
S. Shirobokov, A. Ustyuzhanin, A. Güneş Badyin et al., arXiv:2002.04632

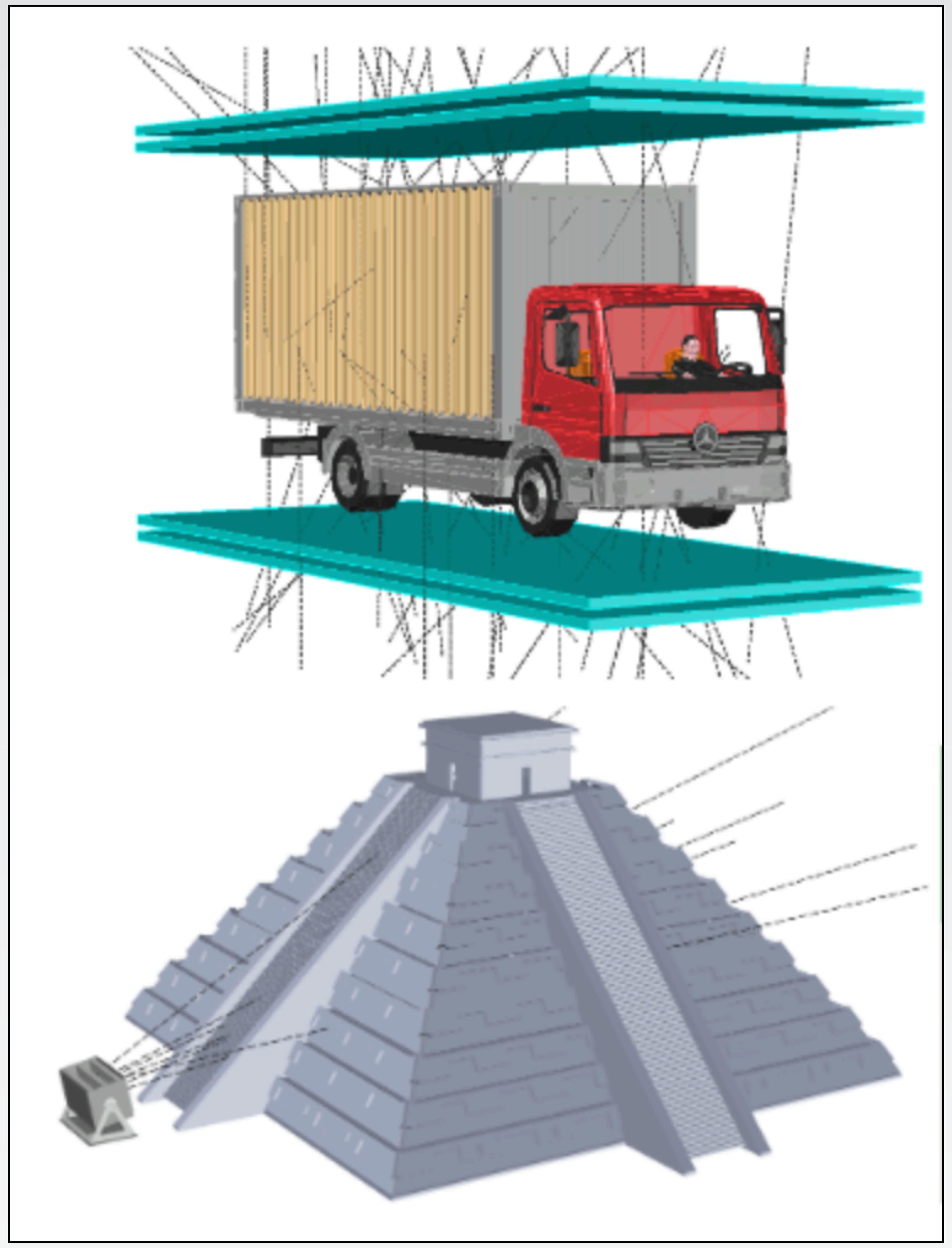
Writing a differentiable simulator: TOMOPT

- Atmospheric muons: 1/s/hand area
- Interact only sparsely with material
- Are scattered enough to be used for imaging applications

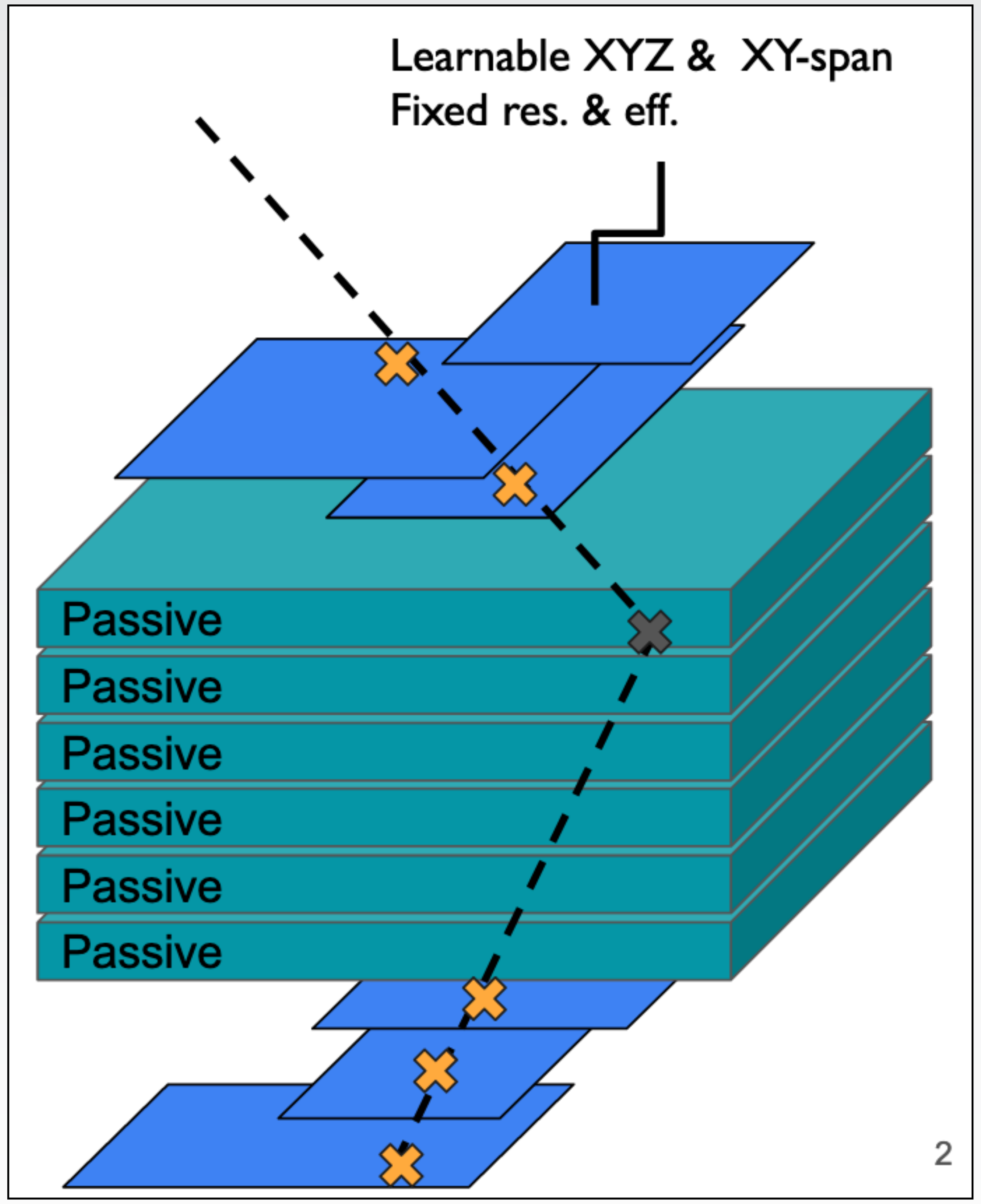
- Detectors: usually panels, with spatial resolution and detection efficiency
- Optimal starting point for a differentiable simulation

- TOMOPT: package to optimise muon tomography detectors (work in progress)





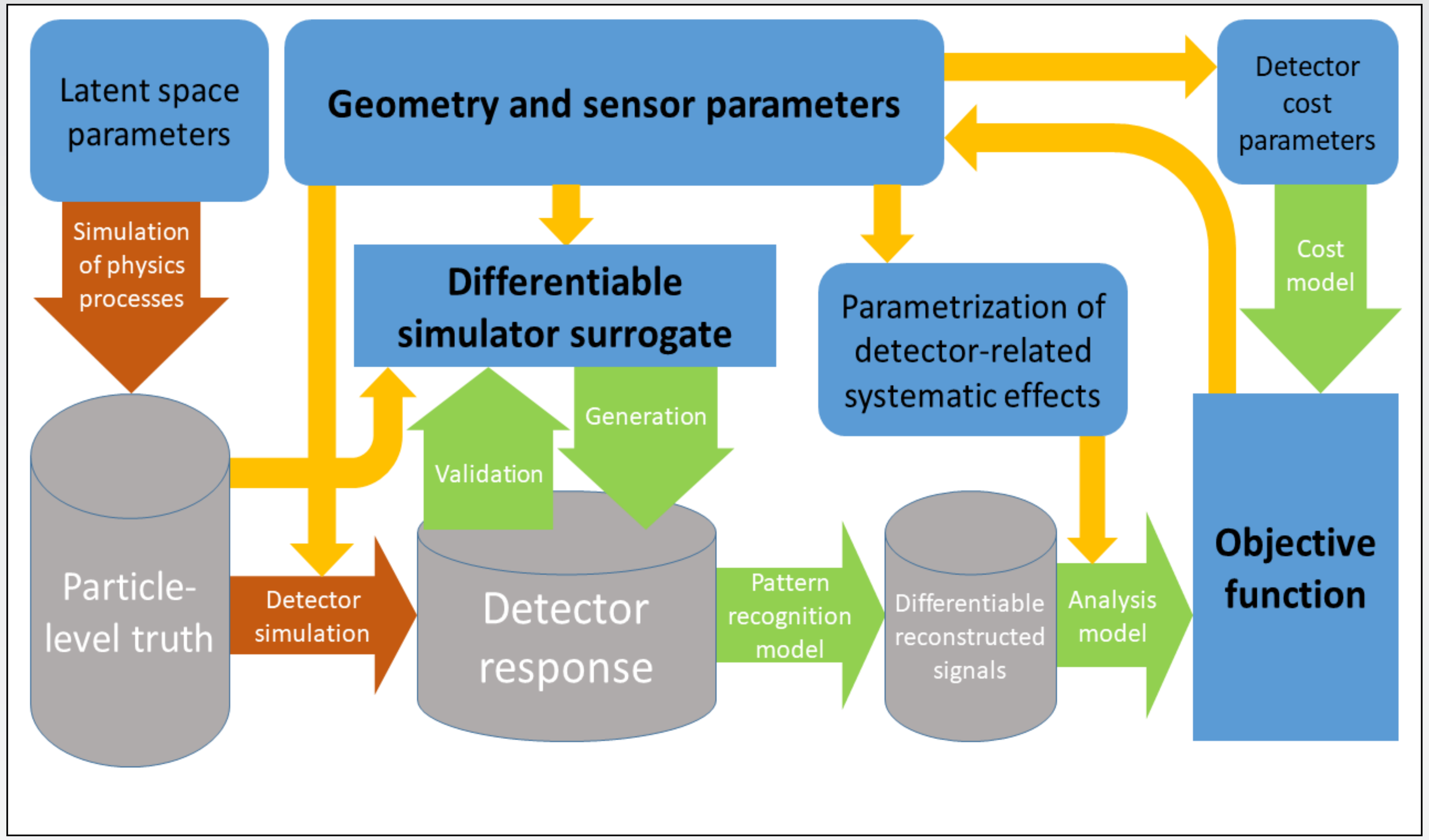
L. Bonechi, R. D'Alessandro, A. Giammanco
arXiv:1906.03934



Work in progress; G. Strong et al.

MODE

- The target of MODE is to design and offer to the community a scalable, versatile architecture that can provide end-to-end optimisation of particle detectors, proving it on a number of different applications across different domains.



- Study cases:
  - **Use known detector concepts in a new way**: demonstration of muon energy measurement in calorimeter
  - **Optimise starting from 'simple' applications** Muon tomography detector optimisation in progress
  - **Rethink decades old paradigms:** Hybrid calorimeter design integrating tracking layers activity starting

- Other use cases being considered / about to start include:
  - Hadron therapy
  - Muon collider detector shielding

- **The developed architectures for optimisation are modular**
  - recycle part of the work for one application when moving to the next one
  - Very happy about any suggestions / contributions

Dear Colleagues,

Initiated by the European Committees for Astroparticle (APPEC), Particle (ECFA) and Nuclear Physics (NuPECC), and following a first joint seminar held in Orsayin 2019, Expressions of Interest for common activities have meanwhile been endorsed in the following areas:

- Dark Matter (iDMEu)
- Machine-learning Optimized Design of Experiments (MODE)

MODE Collaboration, "Toward Machine Learning Optimization of Experimental Design", Nuclear Physics News International, 2021.