Summary of First EuCAIF Conference 2024

Lorenzo Moneta

(SFT Meeting May 27, 2024)

EUROPEAN AI FOR FUNDAMENTAL PHYSICS CONFERENCE
EuCAIFCon 2024

EuCAIF Conference (*30 April - 3 May 2004*)

- First **European AI for Fundamental Physics Conference** (EuCAIFCon)
  - **EuCAIF**: new European initiative for advancing the use of Artificial Intelligence (AI) in Fundamental Physics.
  - **Joint initiative** from particle physics, astroparticle physics, gravitational wave physics, cosmology, nuclear physics and theoretical physics.

JENAA
Joint ECFA-NuPECC-APPEC Activities

- Goal is to **establish connections** between different branches of EuCAIF
- Cross-disciplinary sessions centred on specific AI themes
- Events supported also by

CERN and NexTGen Next Generation Triggers

Conference Organisation

- Organised with plenary sessions, panel discussions, parallel sessions with oral talk and lighting talks
    - Lightening talks presenting also a poster (2 poster sessions)
- **Well organised** with long breaks allowing time for discussions.
    - Large number of participants (more than 200)
        - from students and early career researchers to seniors
- **Great location,** Amsterdam, in a nice Hotel with lunches provided for the 4 days (from Tuesday to Friday)
    - Reasonable conference fees
- See timetable and contributions at conference Indico page.

Plenary presentations

- **Reviews of AI** in the different disciplines
  - Theoretical physics
  - Experimental particle physics
  - Nuclear Physics
  - Gravitational Wave physics
  - Cosmology
  - Astro-particle Physics
- Special keynote talks
  - Methods in AI for Science (*François Charton*)
  - AI ethics and fundamental physics (*Savannah Thais*)
  - Prospects for AI in physics and astronomy (*Max Welling*)
- Closing Keynote Talk:
  - AI for fundamental physics (*Kyle Cranmer*)

Parallel Sessions

- **Large number of contributions** (~ 200)
- Parallel sessions on these topics and number of contributions:
  - Pattern recognition and image analysis (37)
  - Generative models and simulation of physical systems (23)
  - Simulation-based inference (28)
  - Hardware acceleration and FPGA (19)
  - Explainable AI (10)
  - Foundation models and related techniques (12)
  - Physics-informed AI and integration of physics and ML (13)
  - Uncertainty quantification and others (24)
- **Working group discussions**

EuCAIF Working groups

- Foundation Model and Discovery
- Hardware and Design Optimisation
- Fairness and Sustainability
- JENA WP 4 (ML Computing Infrastructure)
- Community connections and funding

Started initial discussion in the working groups

- Define goals and objectives
- Inviting interested members to participate
- Follow-up meetings will better define the future plans

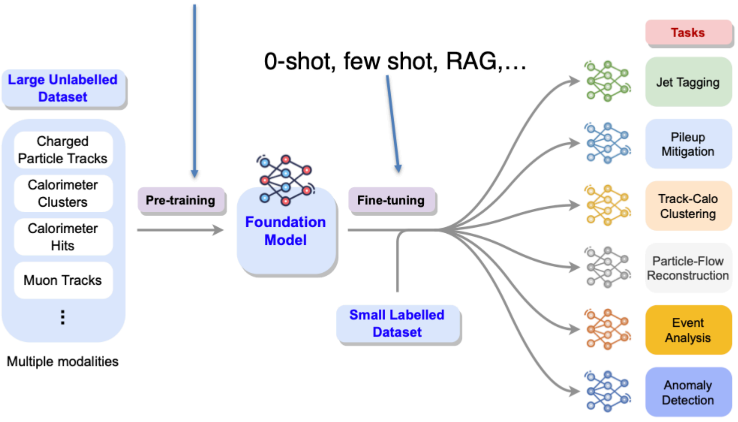
WG1 - Foundation models

- Goals:
  - Facilitate research on large-scale foundation models (FMs) for fundamental physics
  - Provide infrastructure, resources, data and models, connect researchers, define problems & metrics

The Vision

SSL, tokenization, transformers (& beyond?), (flexible) inductive bias?...

0-shot, few shot, RAG,...



More to do:

- More features
- Scale up 100M →10B…
- Multi-modal & -scale
- Common latent space (align?)
- Language modality?
- Adopt industry models to physics
- FM → agents of experts
- Interpretability
- Explore & exploit (→ experiment)

sign up: https://bit.ly/eucaifcon24-wg1

WG 4: White paper for JENA WP4

- Define Machine Learning and Artificial Intelligence Infrastructure
  - define computing requirements for the next decade (JENA computing initiative)
- Mandate of the group:
  - Follow the technologies in this fast evolving field.
  - Analyse the potential impact on the ENA computing infrastructure needs.
  - Quantify the resource needs and define the interfaces and services that are needed by physicists to run ML workloads (looking at both training and inference).
- Timescale: White paper ready by end of the year
- Join the working group:
  → https://indico.scc.kit.edu/event/3813/

Panel Discussions

- Directions AI and fundamental physics
- AI Infrastructure
- Building a European Coalition for AI in Fundamental Physics

Plenary Presentations

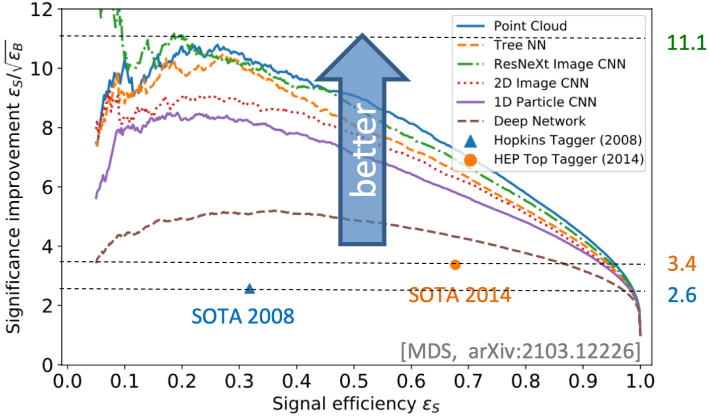
- personal summary of some interesting plenaries (not complete)

Theoretical high-energy physics and AI (*Matthew Schwartz*)

Very interesting and fascinating talk (see slides)

- **Past:** collider physics
- **Present**: symbolic AI for theoretical physics
- Large Language Models show good capability for symbolic problems
    - Example: simplify computation of Feynman diagrams (polylogarithms)
    - approach based on reinforcement learning or transformers
    - Same approach can be used to other problems:
        - Simplifying spinor-helicity amplitudes
        - scattering amplitudes
- ML application also in string theory
- **Future: can machines do theoretical physics?**

Top Tagging (2008 – 2022)



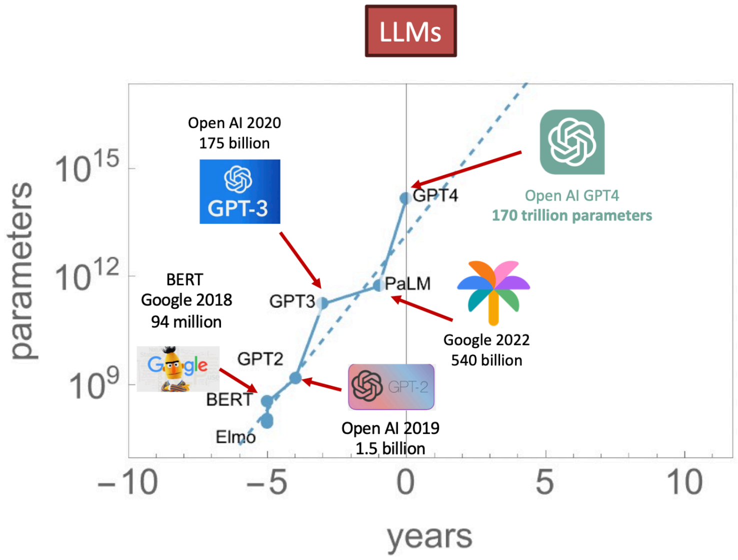
$$f(x) = 9\left(-\mathrm{Li}_3(x) - \mathrm{Li}_3\left(\frac{2ix}{-i+\sqrt{3}}\right) - \mathrm{Li}_3\left(-\frac{2ix}{i+\sqrt{3}}\right)\right)$$
$$+4\left(-\mathrm{Li}_3(x) + \mathrm{Li}_3\left(\frac{x}{x+1}\right) + \mathrm{Li}_3(x+1) - \mathrm{Li}_2(-x)\ln(x+1)\right)$$
$$-4\left(\mathrm{Li}_2(x+1)\ln(x+1) + \frac{1}{6}\ln^3(x+1) + \frac{1}{2}\ln(-x)\ln^2(x+1)\right)$$

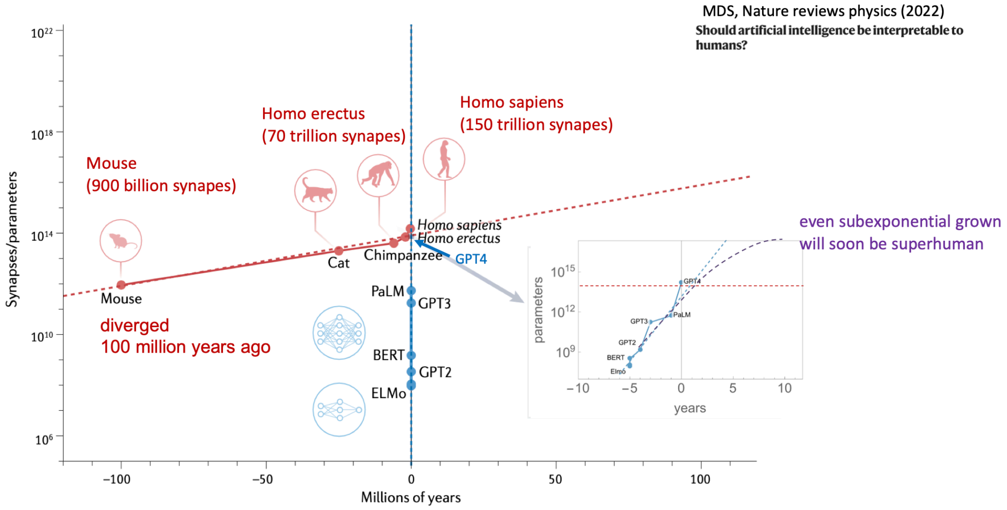
$$f(x) = -\mathrm{Li}_3(x^3) - \mathrm{Li}_3(x^2) + 4\zeta_3$$

Future

LLM are the immediate future

- Biological intelligence grows by a factor of 2 in one million years
- Machine intelligence grows by a factor of 10 in 1 year

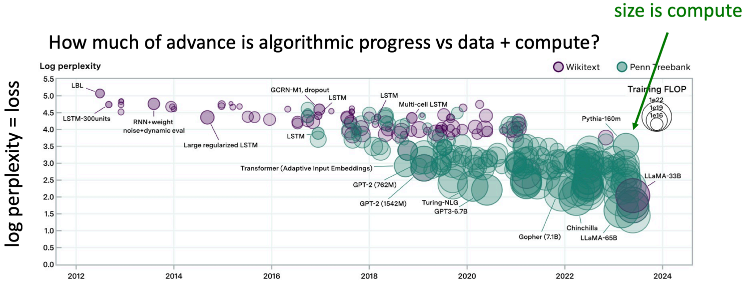




- Both AI and biological intelligence grow exponentially
- **Factor of 10^6 difference in *exponent***
- Intersection, when machines and biology have comparable "intellegence" is now

ALGORITHMIC PROGRESS IN LANGUAGE MODELS

Ho et al. arXiv:2403.05812



algorithmic doubling time = 6 to 14 months!

Some interesting questions

- Physics requires creativity. **Is AI creative?**
  - GPT4 more creative than 99% of humans
- Augmented intelligence: **can AI be a skill-leveler for high-energy physics theory**?
  - with AI average physicist can become as Einstein
- **Theoretical physics may have stalled in recent years**
  - problems are maybe too difficult for humans
    - humans can handle only 5-9 concepts at once and like to visualize
      - computers can handle much more complexity
    - Example: **could a cat ever learn to play chess?**
- Language models are vey close to training themselves to be better physicists
- **Suppose a machine understands the theory, do we need to understand it too**?

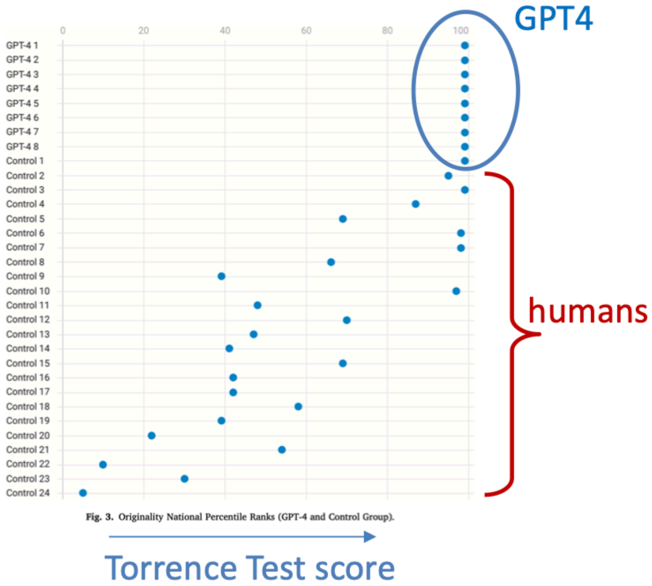


Fig. 3. Originality National Percentile Ranks (GPT-4 and Control Group).

Conclusions

- Machine learning is **rapidly tranforming high energy physics**
  - Current revolution in applications and advances are in "data science"
  - In hep-th and hep-ph problems are largely symbolic

1. How do we transition from data science to symbolic theoretical physics?

- It will get easier once we get started
  - Symbolic search problems (polylogarithms, spinor helicity)
  - Properties of the S-matrix (unitarity)
  - String Theory Vacuua

} searching for simplicity

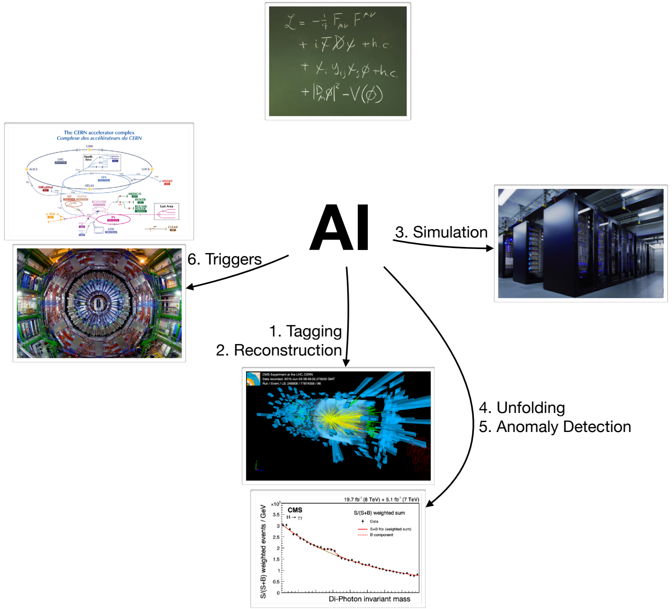
2. Generative AI is the future

- Short term: augmented intelligence
  - Machines help us organize information
  - Smooth transition to arXAIv: more and more AI input into arXiv papers

- Long term: artificial intelligence
  - Machines will suggest problems, solve problems: G Ph. T
  - Machines will dumb things down, so we can appreciate their work
  - Superhard problem in theoretical physics may finally be solved

Experimental particle physics and AI (*Gregor Kasieczka*)

- Role of AI is in experimental particle physics
- Very detailed and complete review (see slides).

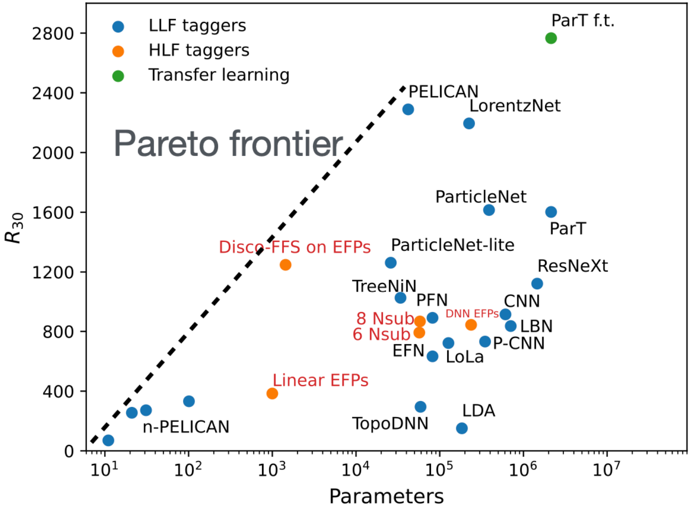


1. **Taggers**
2. **Reconstruction**
3. **Simulation**
4. **Unfolding**
5. **Anomaly Detection**
6. **Triggers**
7. **Inference (SBI)**
8. **Experimental Design**

1. Taggers

Take aways

- Point clouds as powerful paradigm to represent data
- Additional structure in architecture boosts performance
- Over wide range: Best complexity/performance trade-off by physics-informed models
- Overall highest performance reached via transfer learning



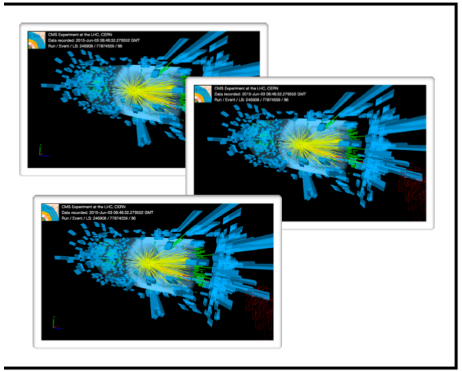
Challenges

- Calibration (domain adaptation: from simulation to collider data)
- uncertainty aware training
- Interpretability

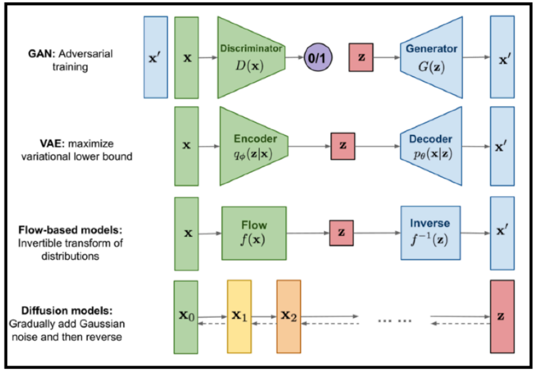
3. Simulation

Strategy

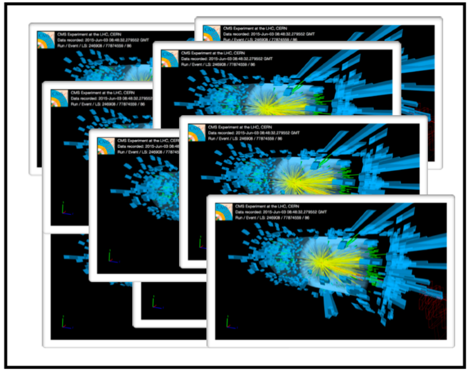
1. Use classical simulation or collider data as input



2. Train generative surrogate



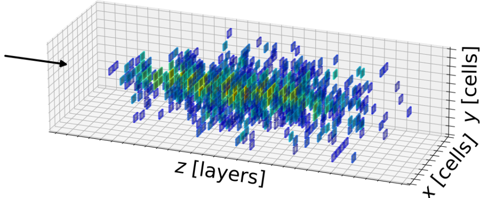
3. Oversample



Main Targets

- Event level kinematics
- Jet constituents
- Calorimeter showers
- pile-up interactions

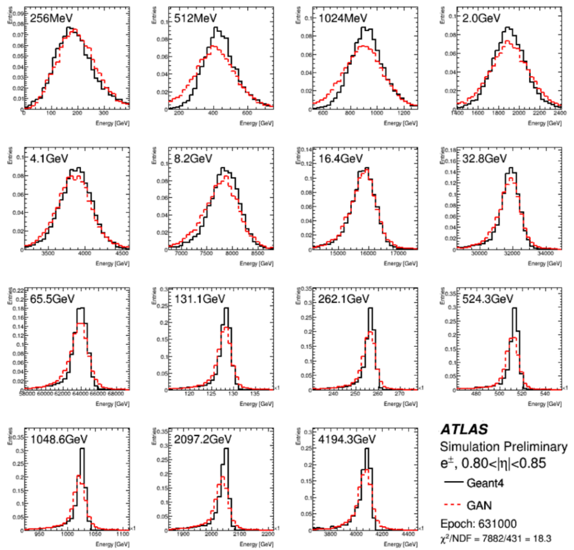
Fixed Grid vs **Point Cloud**

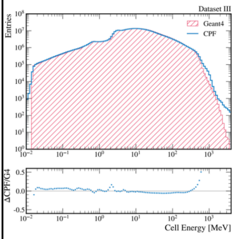


Example: CaloClouds using diffusion

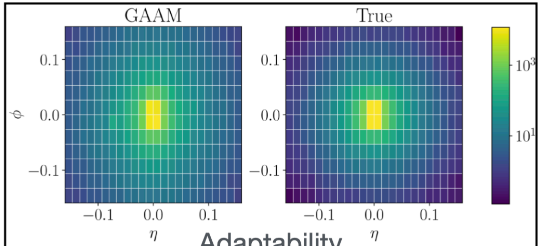
3. Simulation

- **Application**: used in ATLAS (FastCaloGAN in ATLFAST3)
- **Future outlook**:
  - Importance of public datasets to compare algorithms (e.g CaloChallenge 2023)
- Some challenges:
  - Quality of generation
  - Complexity of samples
  - Integration in Geant4
  - Adaptability





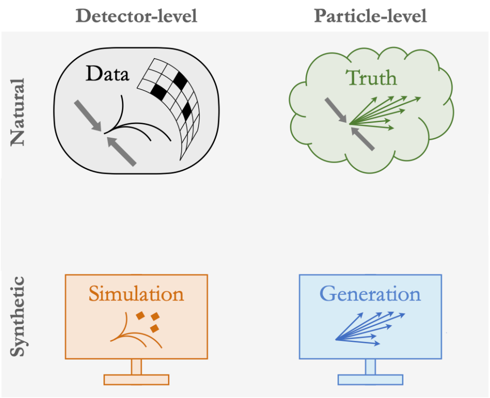
Quality of generation

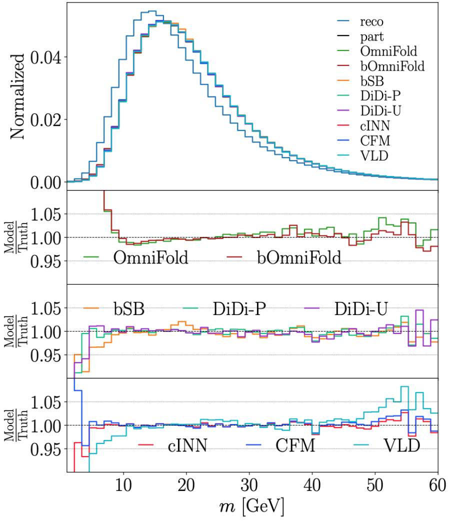


Adaptability

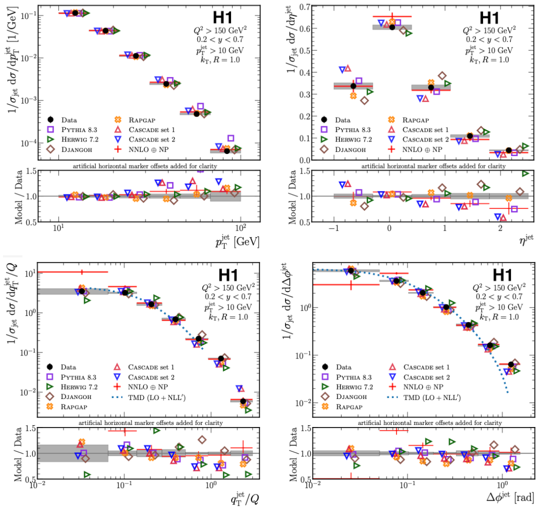
4. Unfolding

- 2 approaches:
  - Reweighting based on classifiers
  - Morphing based on diffusion or generative models





Example: Unfold Z+jets distributions in six dimensions

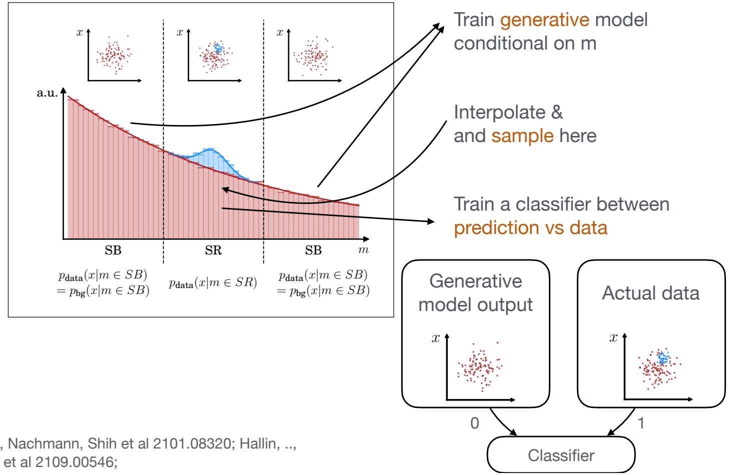


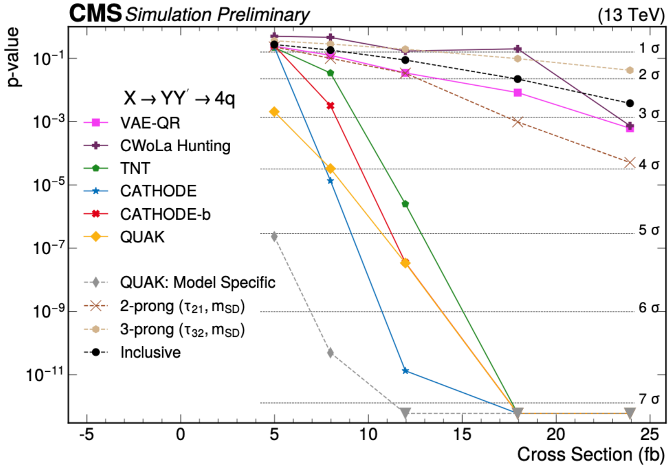
Already applied to collider data: Lepton/jet event at H1

5. Anomaly Detection

- Model independent search of new physics
- CATHODE and CASE (CMS Anomaly Search Effort)

CATHODE



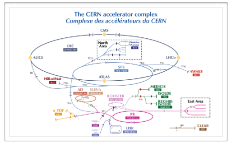


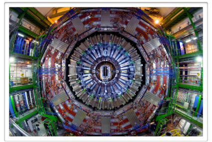
GK, Nachmann, Shih et al 2101.08320; Hallin, ..,
GK et al 2109.00546;

6 Anomaly detectors in parallel using full Run 2 data

6. Trigger

Trigger

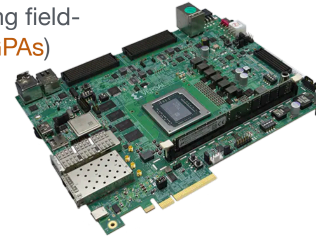




Colliders with
40 million events/second

2 stage system (Trigger) reduces this to ~1 kHz for offline storage and analysis

Stage 1: Hardware based, using field-programmable gate arrays (FGPAs) with microsecond latency



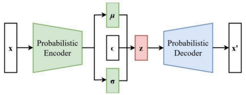
Improving selection criteria in trigger with AI yields better offline data

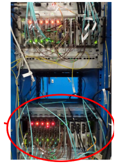
hls4ml to translate ML architectures to hardware language

https://fastmachinelearning.org/

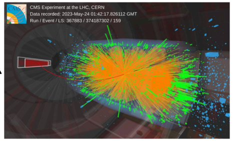
Example: Triggering Outliers

Learn-compression/decompression on signal free sample and use as anomaly score
Now testing in CMS Level 1 trigger



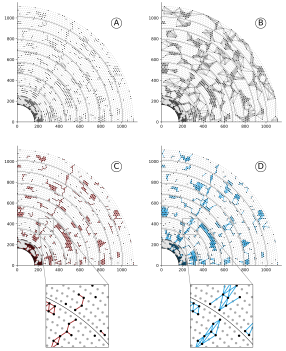


https://indico.cern.ch/event/1283970/contributions/5554350/attachments/2720710/4727877/axol1tl_fastml.pdf



Testing in CMS L1 Trigger

Example: Online graph building



Online graph building for reconstruction in Belle 2 drift chamber

Explore different methods of constructing graphs for GNN processing

Within resource constraints

No. of Vertices	No. of Edges	Width of Edge	Registers abs.	Registers %	LUTs abs.	LUTs %	F7Muxes abs.	F7Muxes %
498	2305	60 bit	145 333	7.84 %	19 370	2.09 %	5760	1.15 %
786	3649	60 bit	246 511	13.30 %	31 360	3.39 %	9120	1.81 %
978	4545	40 bit	206 573	11.15 %	34 252	3.70 %	11 360	2.26 %
978	4545	60 bit	304 919	16.46 %	38 968	4.21 %	11 360	2.26 %
978	4545	100 bit	485 473	26.20 %	47 642	5.14 %	11 200	2.23 %

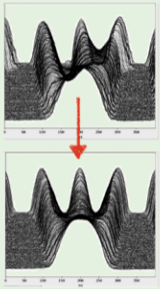
For Belle 2

Neu et al 2307.07289

Accelerator Physics and AI (*Verena Kain*)

- **Using AI for accelerator complex at CERN**
- CERN accelerator complex very diverse, many different types of beams and production schemes
    - current beam scheduling has severe impact on efficiency in running accelerators
    - hysteresis limiting also accelerator efficiency
- Future accelerators (like FCC) need to be run as an autonomous system
- Some Current example of AI usage in accelerators:
    - Bayesian Optimisation for control and optimisation of accelerator
        - ada[tive contínuos control for extracted spill in NA
    - **Reinforcement Learning (RL)**
        - problem online training often not possible (need accurate simulation, e.g. digital twin)

Example: RL at CERN



PS

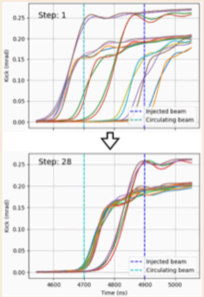
- Correct RF **phase & voltage** for **uniform bunch splitting** (LHC beams)
- Successful **sim2real** & fully **operational**
- **Multi-agent** (SAC) & **CNN** for initial guess
- **Next: continuous** controller (UCAP)

A. Lasheen, J. Wulff

PS to SPS

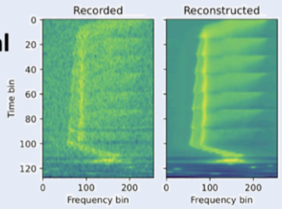
- Adjust **fine delays** of SPS **injection kicker**
- RL agent (PPO) trained on **data-driven dynamics model**
- Ready for **sim2real test**

M. Remta, F. Velotti

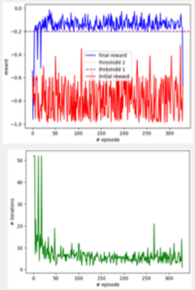


LINAC3 / LEIR

- **PhD project** *(B. Rodriguez)*: control LINAC3 cavities for **optimal injection efficiency** into LEIR
- RL state based on **VAE-encoded Schottky** spectra
- Agent trained on **data-driven dynamics model**



V. Kain, N. Madysa



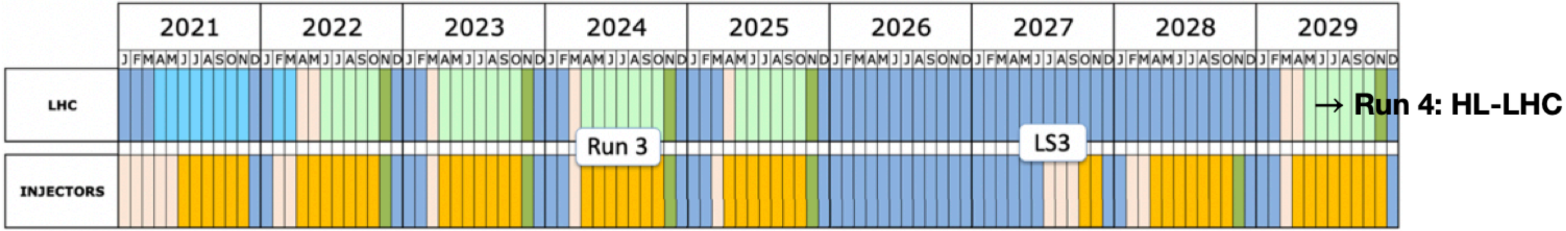
SPS

- **Steer DC beams** in TT20 TL using **split-foil** secondary emission **monitors**
- Works well in simulations, **with noise and varying emittances**
- Ready for **sim2real test**

N. Bruchon, V. Kain

Courtesy M. Schenk

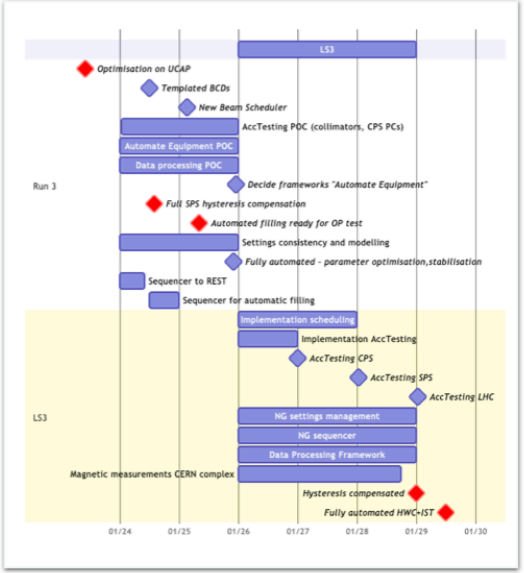
Efficient Particle Accelerators (EPA) project @ CERN



Time bounded project (5 years): improvements ready for **HL-LHC (2029)**

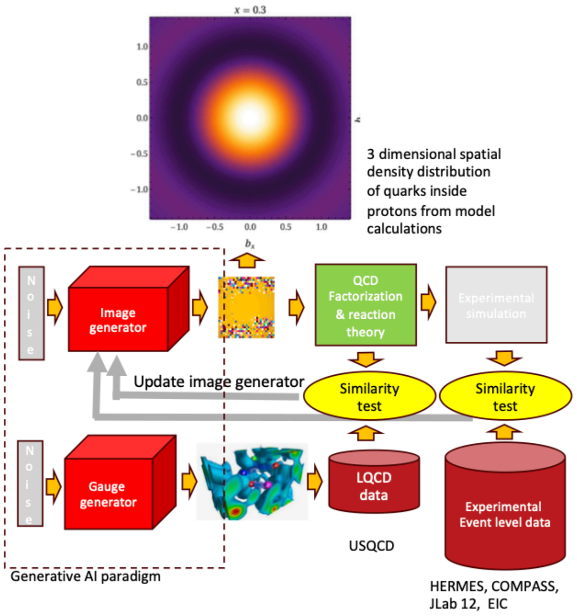
EPA is preparing a new CERN **accelerator exploitation paradigm**

→ **blazing the trail for FCC**



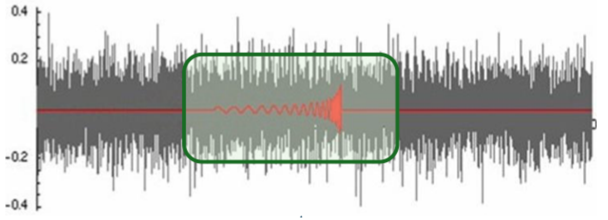
Nuclear Physics and AI (*Amber Boehnlein*)

- AI application in NP, current ones:
  - **Detector Operations**
    - monitoring, experiment control
  - **Reconstruction**
    - standard signal/background discrimination
- Future ambitions:
  - **Detector Design for the Electron-Ion Collider**
  - **Theory/experiment integration**
    - 3D imaging of internal structure of the proton
    - use generative AI for computational nuclear simulation and inverse design problems in nuclear theory



Gravitational wave physics and AI (*Elena Cuoco*)

- Gravitational wave analysis based on detecting a very small signal in a noise-dominated time series
- Use a template description of the signal and then perform Bayesian parameter estimation
- Several places for using AI



NOISE
- Data cleaning
- Glitch classification
- Nonlinear noise
- ITF anomaly detection
- Glitch simulation

BURST
- ML-based method for detection
- CCSN waveform classification

CBC
- Detection
- Early warning
- Anomaly detection

CW
- Clustering in the parameter space
- Computing efficiency

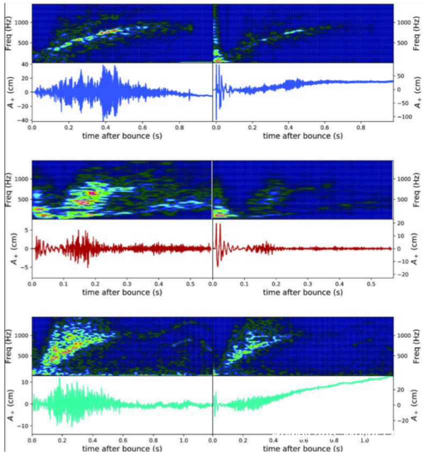
SWBG
- Noise correlation

PARAMETER ESTIMATION
- Faster and efficient methods

ALERT SYSTEM
- Ad hoc hardware/software solution?

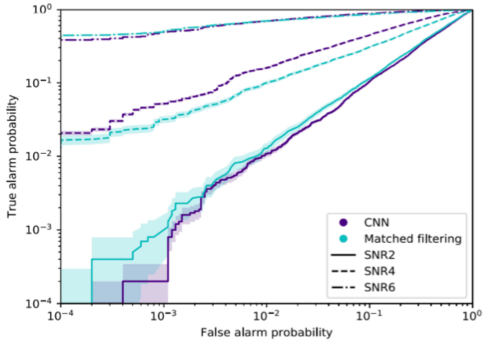
Some examples of AI in GW:

- **Classifying different signals** from core collapsed supernovae (CCSN) using CNN and LSTM (time series is like an image in time-frequency domain)
- **Gravitational Wave modelling**: waveform building using AI (e.g Gaussian process)
- **CBC** (Compact binary coalescence) **detection** using ML
- **Anomaly detection** (using auto-encoder based algorithms)
- **Parameter estimation** using autoregressive normalising flows



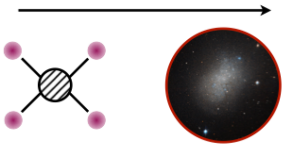
Matching Matched Filtering with Deep Networks for Gravitational-Wave Astronomy

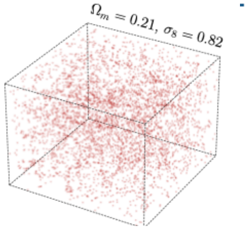
Hunter Gabbard,* Michael Williams, Fergus Hayes, and Chris Messenger
SUPA, School of Physics and Astronomy, University of Glasgow, Glasgow G12 8QQ, United Kingdom

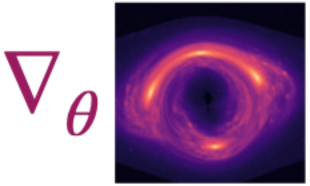


Astroparticle Physics and AI (*Siddarth Mishra-Sharma*)

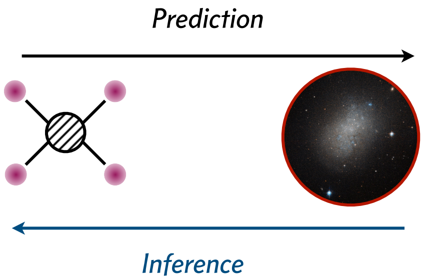
- A large amount of data is coming:
  - e.g. Vera Rubin observatory, Euclid, Next Generation CMB, etc..
- The ability to make robust conclusions is often limited by the challenges in connection theory to data
- Main AI usage:
  - **Simulation-based inference**
    - for inverting complex physical simulators
    - several applications existing
  - **Generative models**
    - for capturing the distribution of complex data
    - used to construct likelihood
  - **Differentiable and probabilistic programming**
    - for specifying models and enabling flexible inference
    - enable end-to-end gradient based optimisation



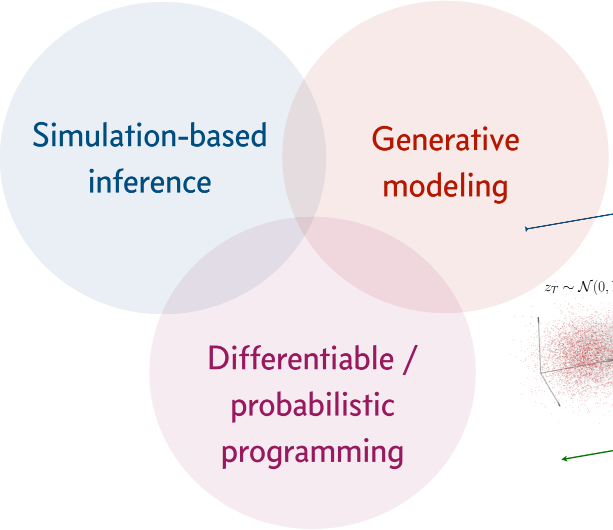




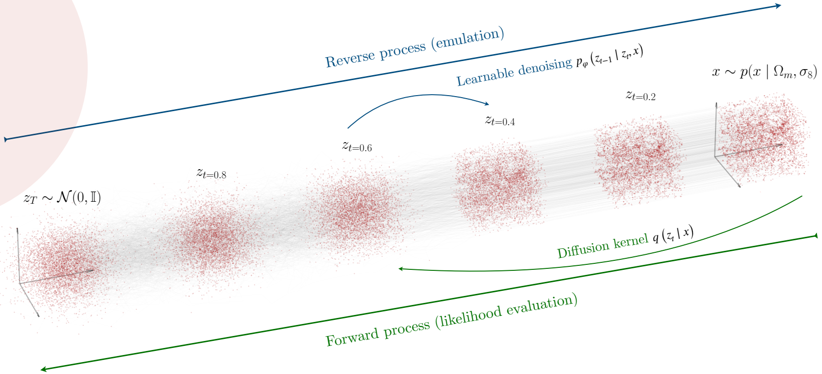
Conclusions

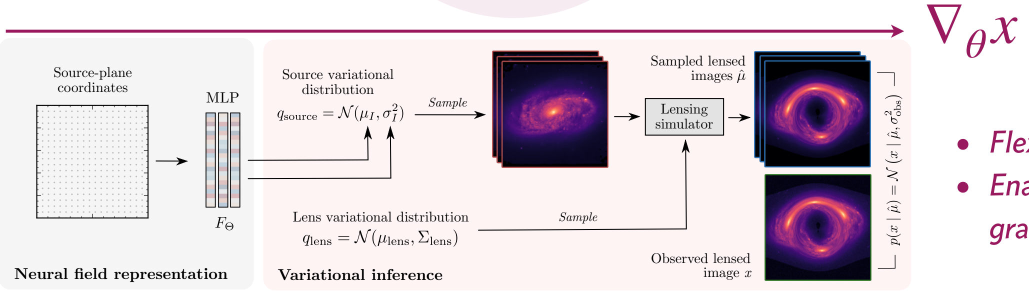


- *Invert complex physical simulators*
- *Directly work with high-dim data*



- *Encode complex physical distribution*
- *Uses end-to-end or as physical priors*
- *Compute data-sim compatibility*





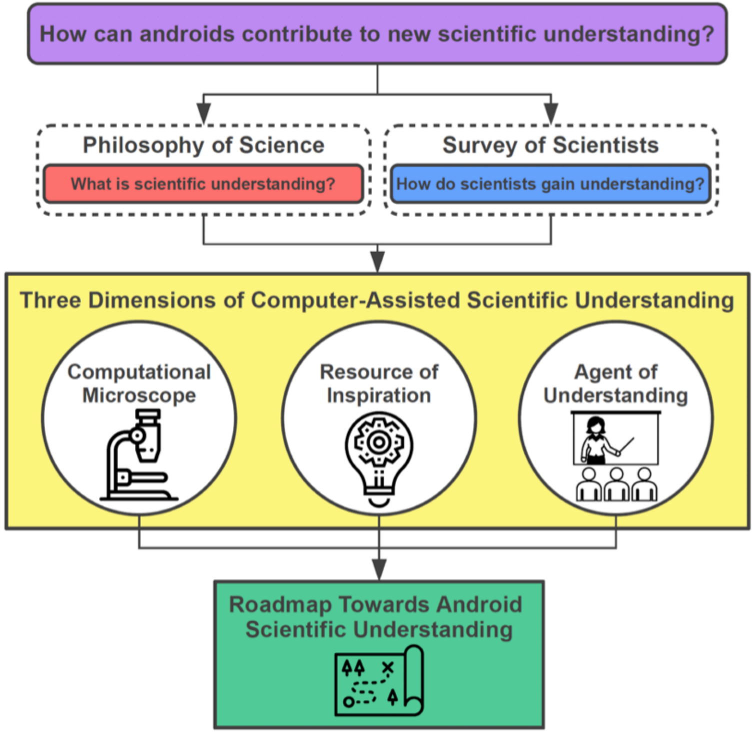
- *Flexible specification of model components*
- *Enable high-dimensional optimization using gradient-based inference techniques*

Final Keynote: AI for fundamental physics (*Kyle Cranmer*)

- **AI/ML as emulators of complex simulations**
- **Scientific understanding**

  How does AI enable or enhance scientific understanding?
    - computational microscope (providing information)
    - resource of inspiration expanding human scope
    - agent of understanding replacing human in generalising observations
        - human less essential here

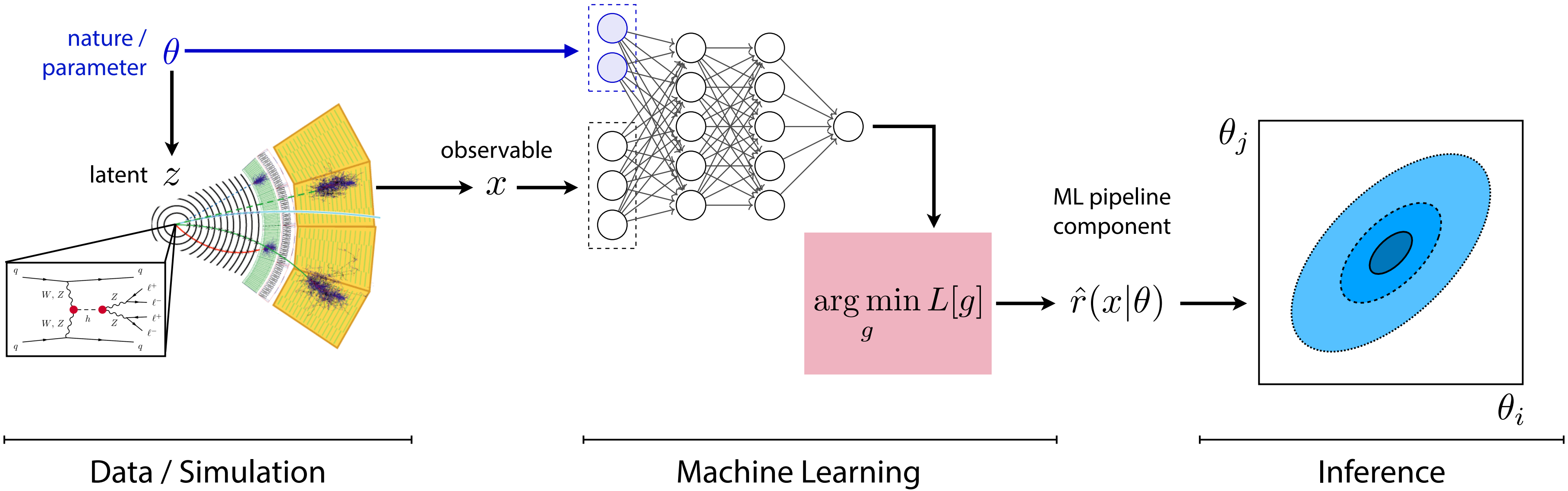
- **Use of ML in Physics vs Molecules & Materials**
    - Many use of AI aimed at material and drug discovery
    - In physics ML is a component in data analysis pipeline
        - **mistakes matter, need uncertainty quantification**



Simulation-Based Inference

Deep learning and neural density estimation are effective at learning approximate surrogates for the likelihood and posterior, **revolutionizing principled statistical inference in science!**

- Removes the need for hand-engineered summary statistics that sacrifice power



Parallel Presentations

- Several diverse contributions especially from students and early career researchers.
- A lot on AI applications on fast simulation, simulation base inference, and pattern recognition

Parallel (Poster) contributions: b-hive (*Niclas Eich*)

- b-hive: a **modular ML training framework** for state-of-the-art object- tagging within the Python ecosystem at the CMS experiment
  - **Full end-end pipeline**: from ROOT file to training ML models
    - Deploying state of the art models (Particle Net, Transformers)
  - Pythonic framework
    - use coffee, awkward and numpy
    - support Tensorflow and PyTorch

see more at CERN-CMS-DP-2024-20

Conclusions

- Great conference with every expert of ML/AI in HEP and fundamental physics.
    - A large number of interesting contributions
    - Good occasion to talk to many people in AI/ML community
    - Thank you for the organisers (*Sacha Caron and Cristoph Weniger)*
- The next conference will be organised next year (in Cagliari, Italy)