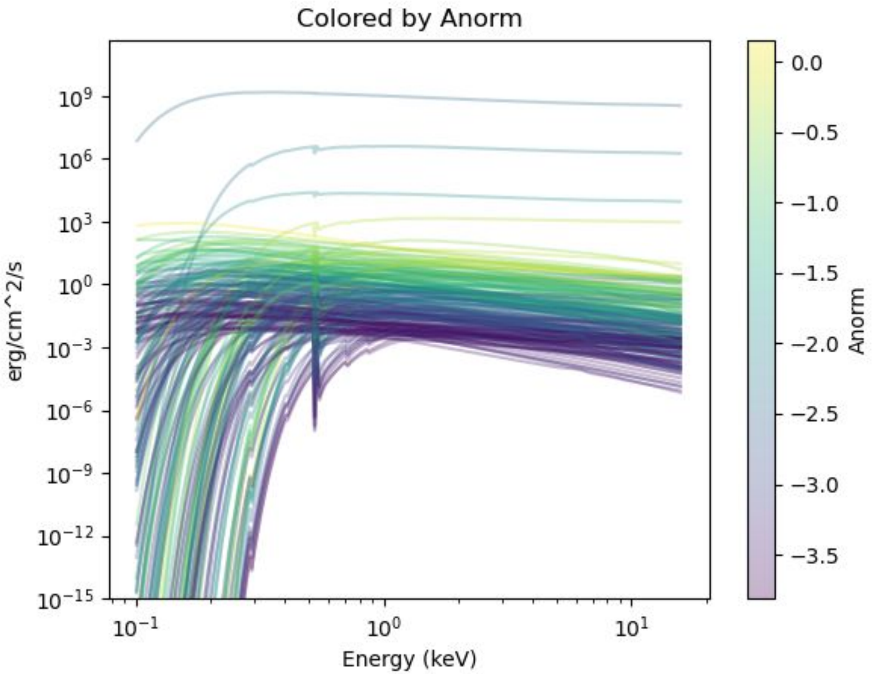
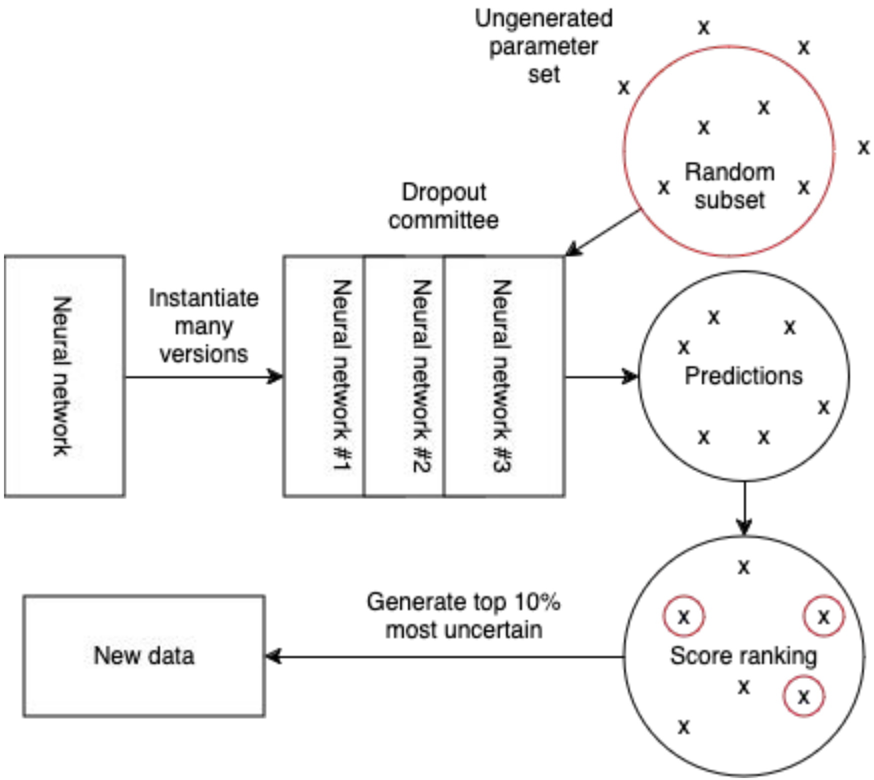
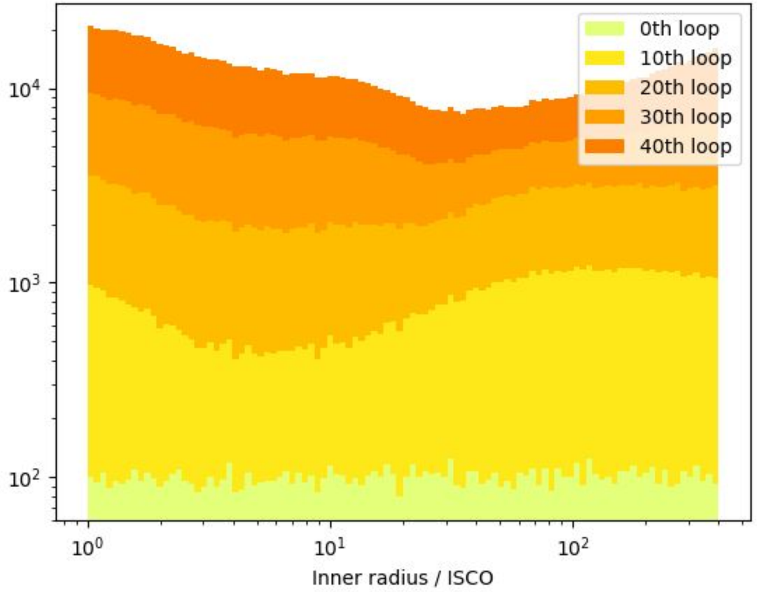
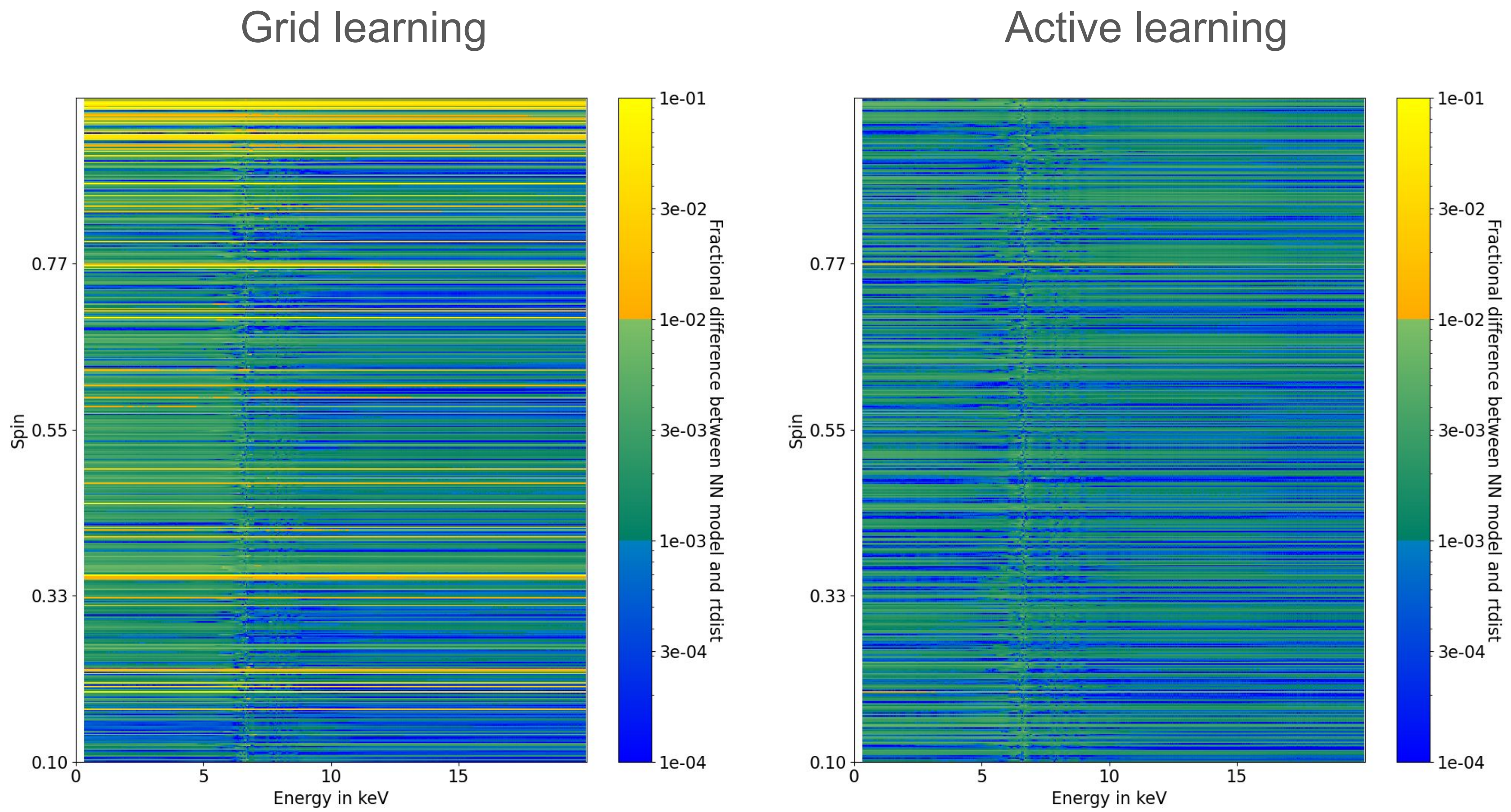
# Emulation by committee: faster AGN fitting



# Query by dropout committee




Grid learning
Active learning
Spin
0.77
0.55
0.33
0.10
0
5
10
15
Energy in keV
1e-01
3e-02
1e-02
3e-03
1e-03
3e-04
1e-04
Fractional difference between NN model and rtdist

# Estimating classical mutual information for spin systems and scalar field theories using generative neural networks

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UNIWERSYTET JAGIELLOŃSKI W KRAKOWIE

Location: 44

*2.2 Generative models & Simulation of physical systems*

# ML enhanced Monte Carlo simulations

## Mutual information

Mutual information quantifies the "amount of information" obtained about one random variable by observing the other random variable. The bipartite partitioning into $A, B$ allows defining the Shannon mutual information as

$$I = \sum_{\mathrm{a,b}} p(\mathrm{a,b}) \log \frac{p(\mathrm{a,b})}{p(\mathrm{a})p(\mathrm{b})}$$

## Ancestral sampling using autoregressive neural networks

We factorize the probability into a product of conditional probabilities

$$p(\mathrm{s}) \;=\; p(s^1)\prod_{i=2}^{N} p(s^i|s^1,\dots,s^{i-1}) \;\approx\; q_\theta(s^1)\prod_{i=2}^{N} q_\theta(s^i|s^1,\dots,s^{i-1}).$$

Using reweighting from $p$ to $q_\theta$ provides us with access to the full partition function $Z(\beta)$ as well as $Z(a,\beta)$ and $Z(b,\beta)$ and write MI as

$$I(\beta) = \log\langle \hat{w}(\mathrm{a,b})\rangle_{q_\theta} - \beta\langle w(\mathrm{a,b})E(\mathrm{a,b})\rangle_{q_\theta} - \langle w(\mathrm{a,b})\log Z(\mathrm{a})\rangle_{q_\theta} - \langle w(\mathrm{a,b})\log Z(\mathrm{b})\rangle_{q_\theta}.$$

## Applications

Our group has applied this approach to various models:

- quantum entanglement in the Ising chain
  ⇒ Dawid Zapolski *Calculating entanglement entropy with generative neural networks*, Location 41
- hierarchical algorithm for the three-dimensional Ising model
  ⇒ Mateusz Winiarski *Applying hierarchical autoregressive neural networks for three-dimensional Ising model*, Location 74
- higher-dimensional Ising model and $Z_2$ gauge model
  ⇒ Vaibhav Chahar *Simulation of $Z_2$ model using Variational Autoregressive Network (VAN)*, Location 1
- Potts model

ÖAW AUSTRIAN ACADEMY OF SCIENCES

HEPHY INSTITUTE OF HIGH ENERGY PHYSICS

# Flow-based generative models for particle calorimeter simulation

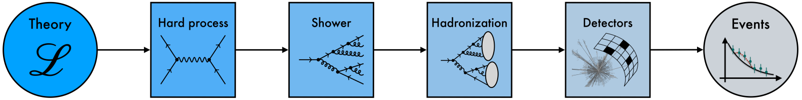
## — EuCAIFCon, Amsterdam, NL —

Claudius Krause

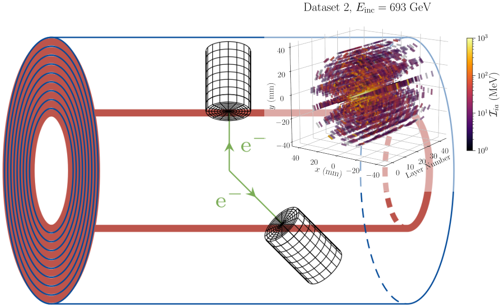
Institute of High Energy Physics (HEPHY), Austrian Academy of Sciences (OeAW)

April 30, 2024

# Our computational ressources are limited!




Machine Learning and LHC Event Generation, A. Butter et al. [2203.07460], R. Winterhalder




We need fast and faithful surrogates.

⇒ Normalizing Flows are both.

latent space ⟵ Bijector, $\mathcal{L} = -\log p$ ⟶ data space

# Flow-based generative models for particle calorimeter simulation

1. Learn how total energy is distributed across layers: $p_1(E_1, E_2, \ldots, E_n | E_{inc})$
2. Learn normalized shower:

- **direct**: learn $p_2(\hat{\mathcal{I}}_{1:n} | E_{1:n}, E_{inc})$
- **autoregressive**: learn first layer $p_2(\hat{\mathcal{I}}_1 | E_1, E_{inc})$ and step from $(n-1)$ to $n$: $p_3(\hat{\mathcal{I}}_n | \hat{\mathcal{I}}_{n-1}, n, E_n, E_{n-1}, E_{inc})$

CaloChallenge datasets

| Dataset | | Method | generation time per shower [ms] ↓ | AUC on voxels ↓ |
|---|---|---|---|---|
| 1: $\gamma$ 368-dim | | GEANT4 | $\mathcal{O}(10^4)$ | 0.499(2) |
| | **d** | CaloFlow IAF | $0.79 \pm 0.01$ | 0.761(2) |
| | **d** | CaloINN | $0.51 \pm 0.03$ | 0.626(4) |
| 1: $\pi^+$ 533-dim | | GEANT4 | $\mathcal{O}(10^4)$ | 0.609(4) |
| | **d** | CaloFlow IAF | $1.00 \pm 0.02$ | 0.884(2) |
| | **d** | CaloINN | $0.44 \pm 0.01$ | 0.784(2) |
| 2: $e^-$ 6480-dim | | GEANT4 | $\mathcal{O}(10^5)$ | 0.500(2) |
| | **a** | iCaloFlow IAF | $13.2 \pm 0.5$ | 0.819(4) |
| | **d** | CaloINN | $1.18 \pm 0.03$ | 0.743(2) |
| 3: $e^-$ 40500-dim | | GEANT4 | $\mathcal{O}(10^5)$ | 0.498(2) |
| | **a** | iCaloFlow IAF | $16.7 \pm 0.5$ | 0.891(3) |

Classify Showers vs. GEANT4 as metric.