FERMILAB-SLIDES-24-0065-CMS-CSAID-PPD

Evolution of Generation and Simulation Techniques in the AI/ML Era

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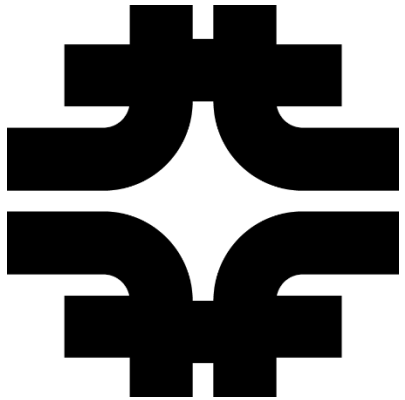
(Fermilab)
April 3, 2024



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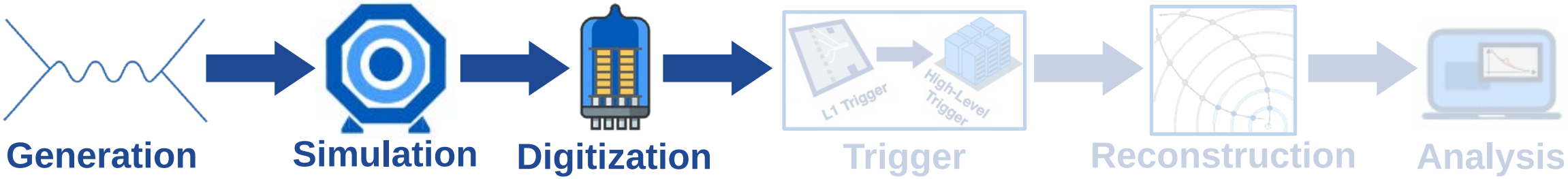
HEP Data Processing & Analysis



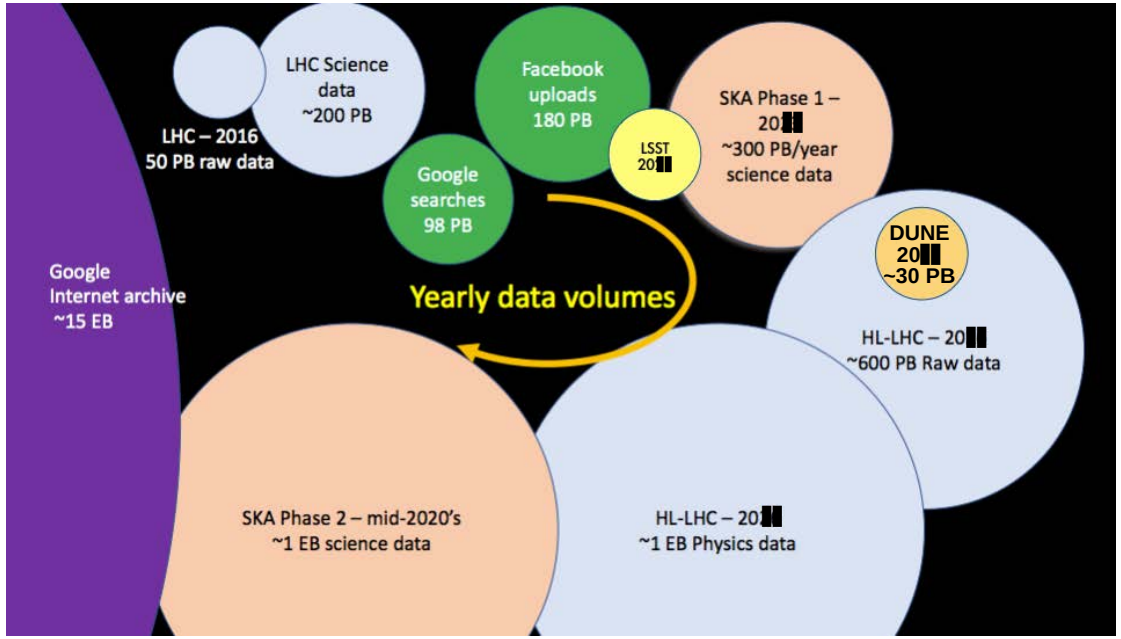
Generation | **Simulation** | **Digitization** | Trigger | Reconstruction | Analysis

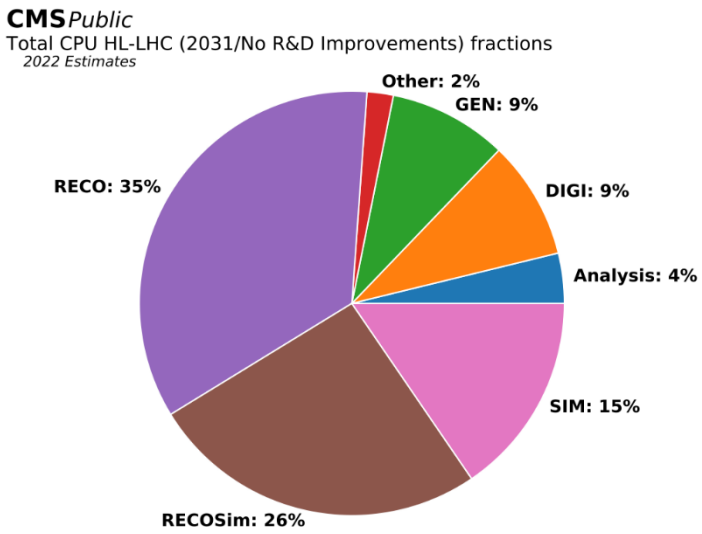
Generation	Simulation	Digitization
Cross section calculation	Geometry navigation	Electronics modeling
Matrix elements (amplitudes)	Material modeling	Pileup
Parton showering, hadronization	Physics interactions	

Somewhat collider-centric view, but conceptually similar in neutrino physics, astrophysics, etc.

- Nearly all HEP results are built on simulations:
  - Detector design, analysis optimization, background estimation, etc.
- As we probe rarer processes, explore more complicated models, and make more precise measurements:
  - Accuracy and computational speed increase in importance!

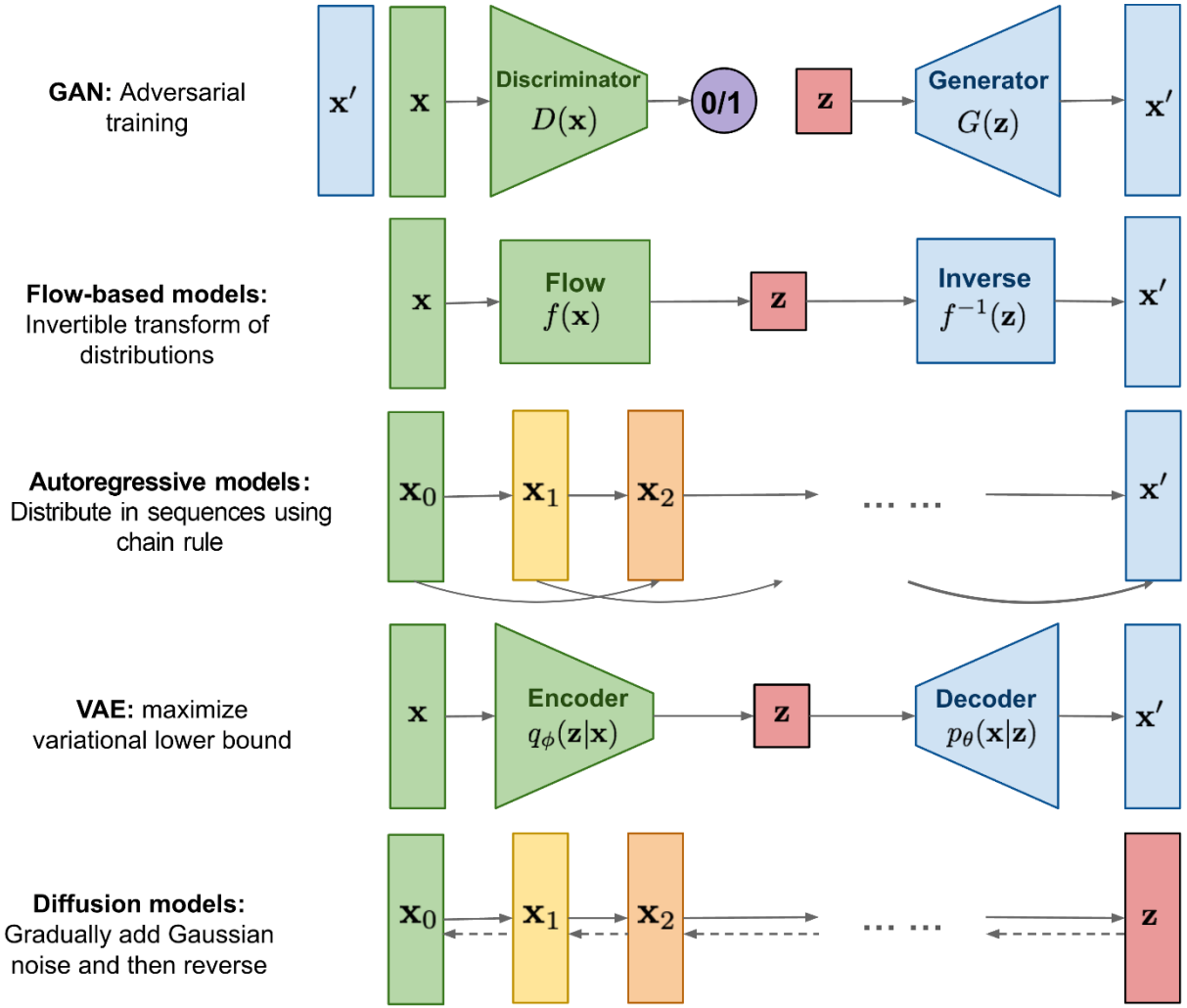
Computing





- A new precision era is imminent: HL-LHC, DUNE, LSST, SKA
  - 10× or more data compared to existing experiments
- **Generation** will need increased fraction of computing for *higher-order calculations*
- **Simulation** needs to deliver more events with more complexity and more accuracy
  - Match growing data volumes and improved detectors… while using *smaller fraction* of computing!
    - To allow for increasing fraction of **reconstruction** (scales *superlinearly* with pileup)

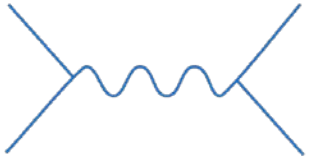
Generative Models



L. Weng

- *Implicit* density estimation: Generative Adversarial Networks (GANs)
  - Pros: fast
  - Cons: can suffer from mode collapse, lack of convergence, etc.
- *Exact* density estimation: Normalizing Flows (NFs), Autoregressive models (ARs)
  - Pros: accurate, fast in one direction
  - Cons: poor scaling, slow in other direction
- *Approximate* density estimation: Variational Autoencoders (VAEs), Diffusion Models (DMs)
  - VAEs: fast, but limited quality
  - DMs: high quality, but slow
- *Non-generative*: reweighting, refinement
  - Classification- or regression-based

Reweighting for Uncertainties

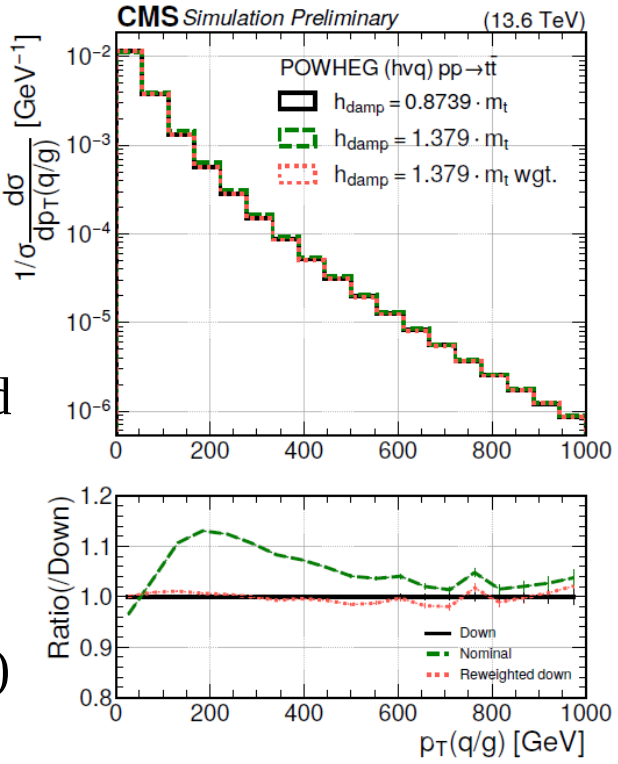


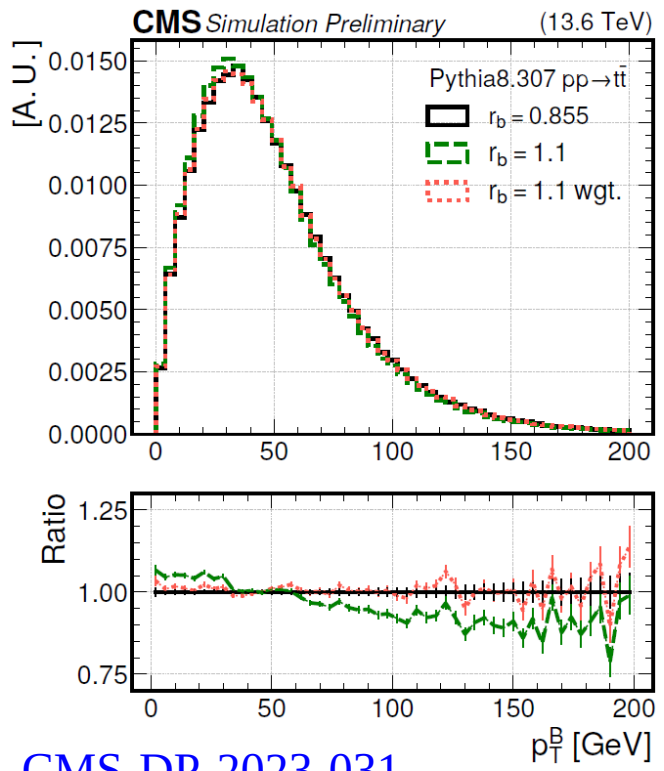
Generation

- Event generators come with many *theoretical uncertainties* in internal parameters
  - Some can be represented as alternate weights for a single event
  - Others cannot; producing multiple samples is extremely computationally demanding (need enough events to minimize redundant statistical uncertainties)
- DCTR method: arXiv:1907.08209
  - Train a classifier C to distinguish between two datasets A & B
  - Then dataset B can be reweighted to the distribution of dataset A using NN output: $w = C(x)/(1 - C(x)) \approx p_A(x)/p_B(x)$
- Train on generator-level information: only need to repeat first step

➢ Effectively transforms all theory uncertainties into event weights!

  - Shown for h_{damp} (POWHEG) & r_b (PYTHIA)
  - Expect rapid adoption!





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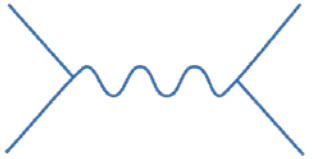
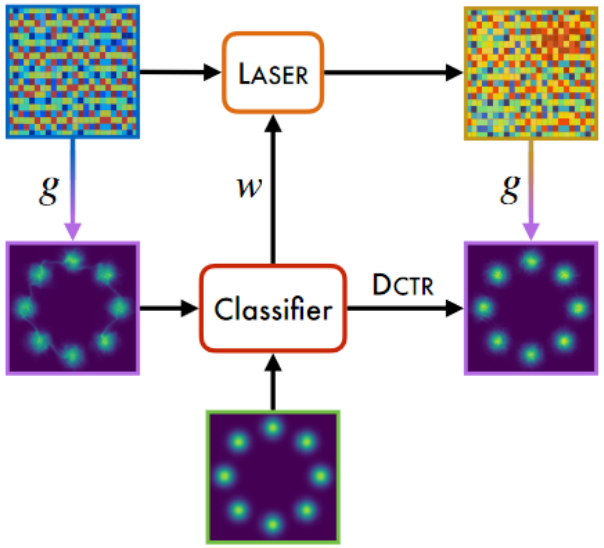
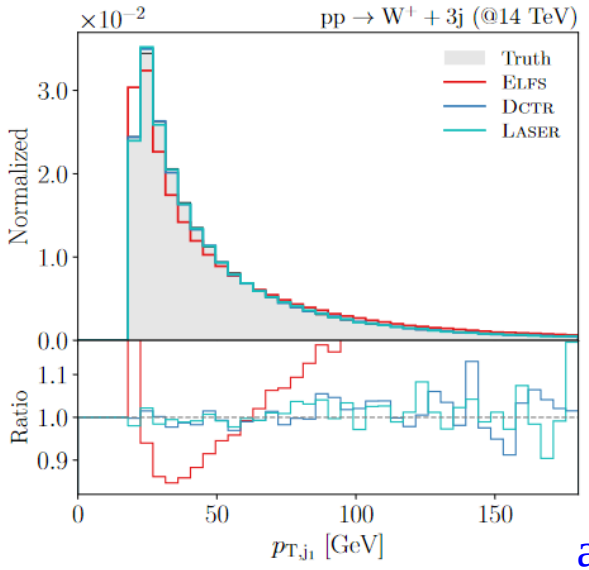
Latent Space Refinement

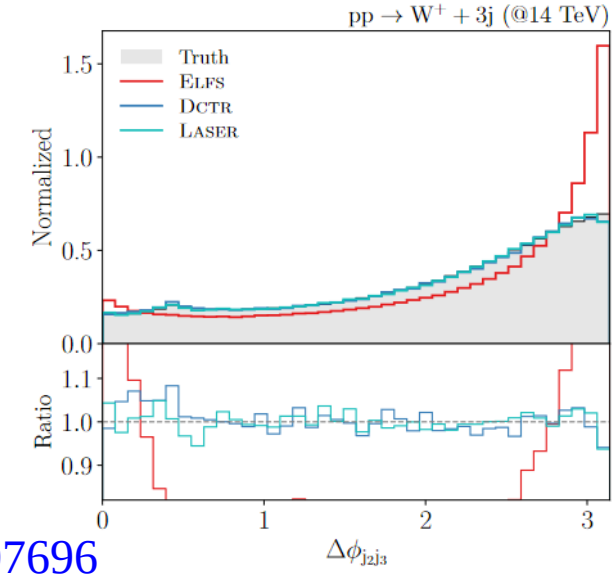


Generation

- DCTR gives accurate output, but reduces statistical precision (events have weights)
- Alternative: apply weights to *latent space* of generative model (NF) → LASER
  - Requires sampling from latent space using Hamiltonian Monte Carlo
- Result: unweighted events with comparable precision to DCTR
  - Promising for important and computing-intensive processes like W+jets
  - Performance also depends on preprocessing of features (particle 4-vectors)







arXiv:2305.07696

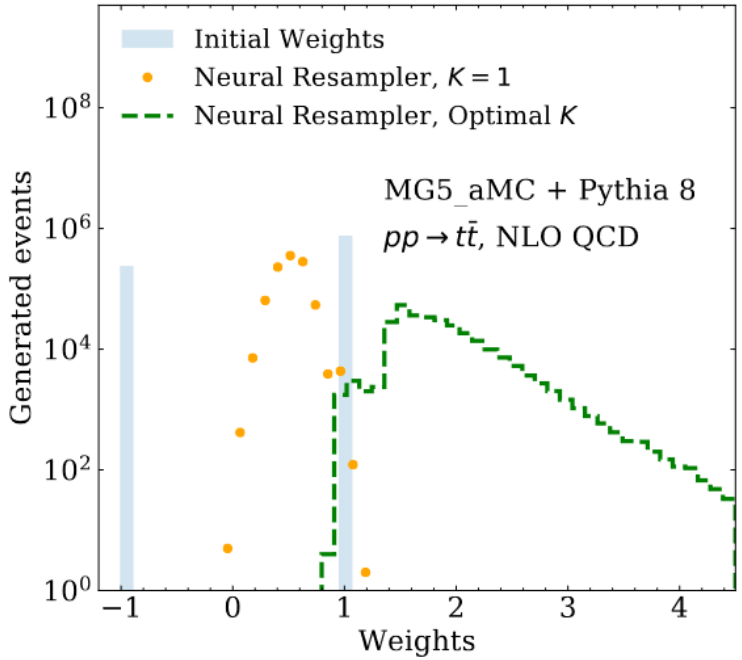
Resampling to Reduce Negative Weights

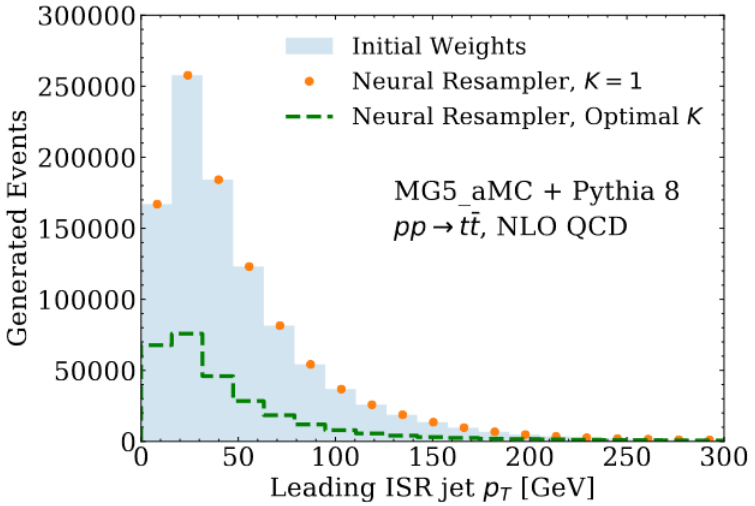
Generation

- Use Particle Flow Network (DeepSet architecture) to learn weight W and variance W^2
  - o Employing DCTR approach
- Define $K = W^2/(W)^2$
- Keep an event with probability 1/K
- Set weights of kept events to be WK

➢ Substantially reduce number of generated events

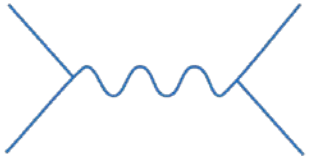
- o *Eliminate* all negative weights
- o Preserve both mean and variance
- o Reduce downstream computational burden:
  fewer events to simulate, digitize, reconstruct, analyze





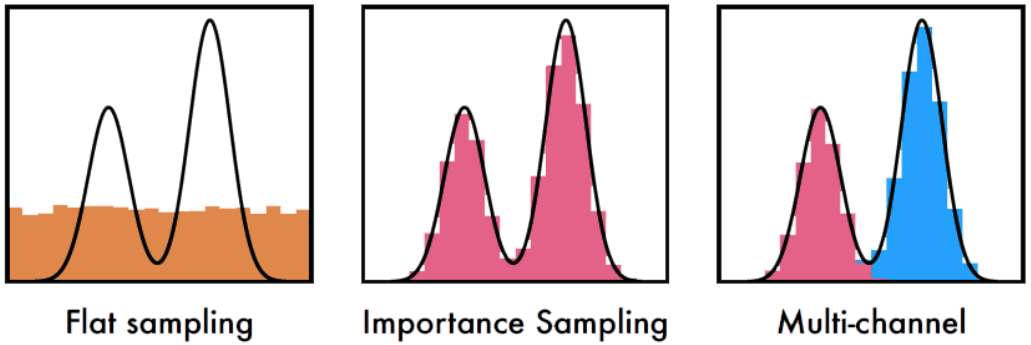
arXiv:2007.11586

MadNIS



Generation

- Expanded use of *neural importance sampling* for multi-channel processes
- Combines generative and non-generative ML
- Implemented in MadGraph
- Substantial improvement especially for processes w/ interference (e.g. vector boson scattering)



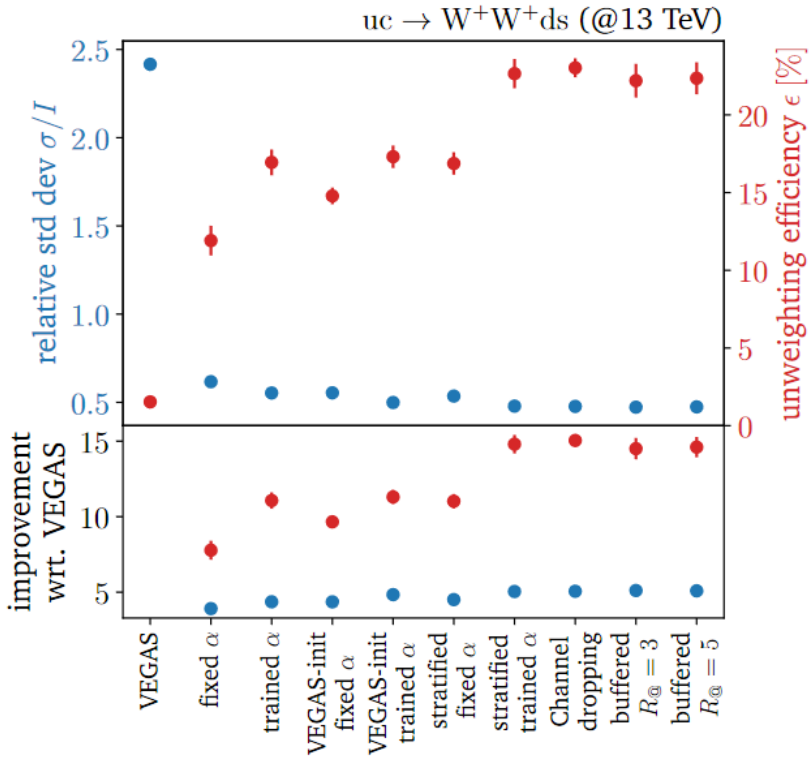
$$I = \sum_i \left\langle \alpha_i(x) \frac{f(x)}{g_i(x)} \right\rangle_{x \sim g_i(x)}$$

Weights: Parametrize with **NN**

Mappings: Parametrize with **NF**

R. Winterhalder

- New methods:
  - Stratified training: more samples for higher-variance channels
  - Channel dropping: remove channels with insignificant weights

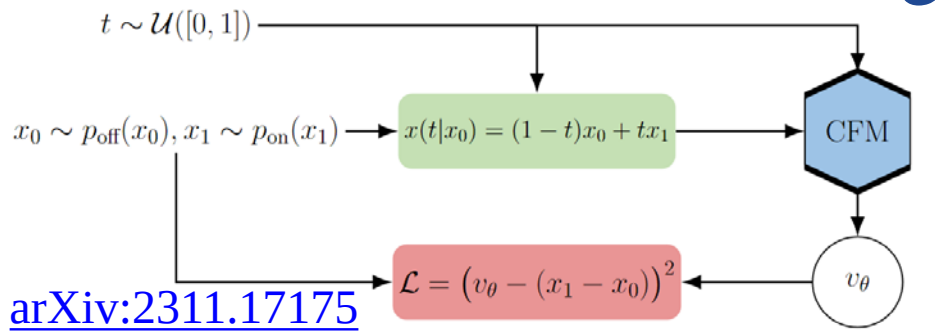


arXiv:2311.01548; see also T. Heimel

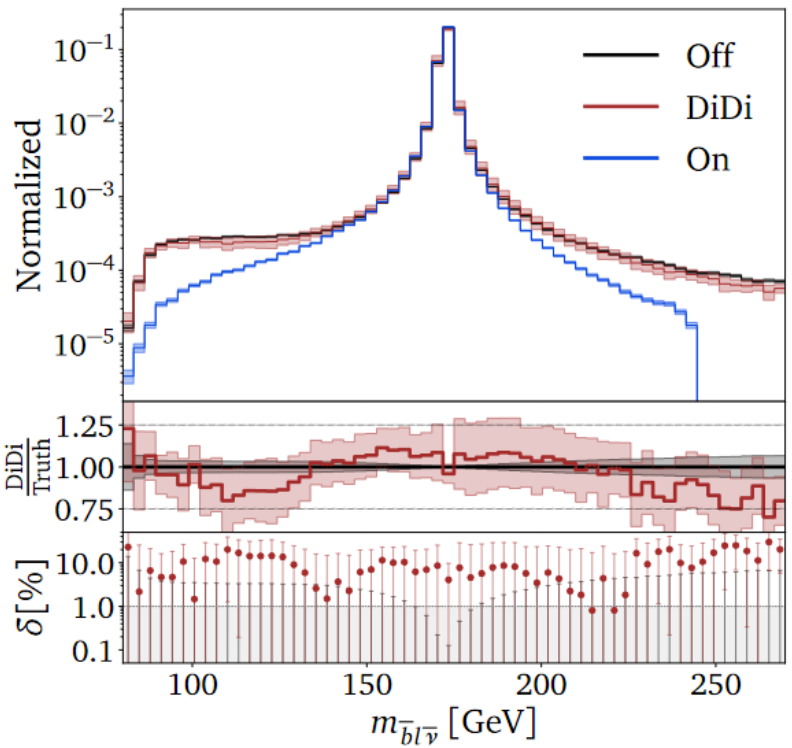
Off-Shell Effects

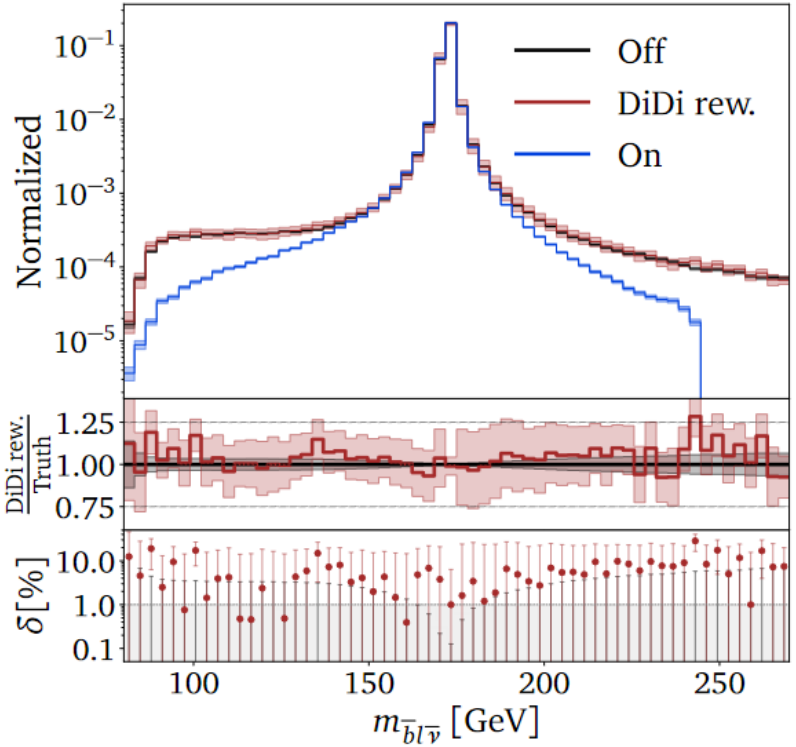
Generation

- Precision measurements require eliminating on-shell approximations
- Direct diffusion (DiDi) model that learns a mapping from on-shell (x_1) to off-shell (x_0) distributions
  - Using conditional flow matching
- Good results for off-shell $t\bar{t}$ production (proof of concept)
- Results can be further improved with DCTR-style reweighting

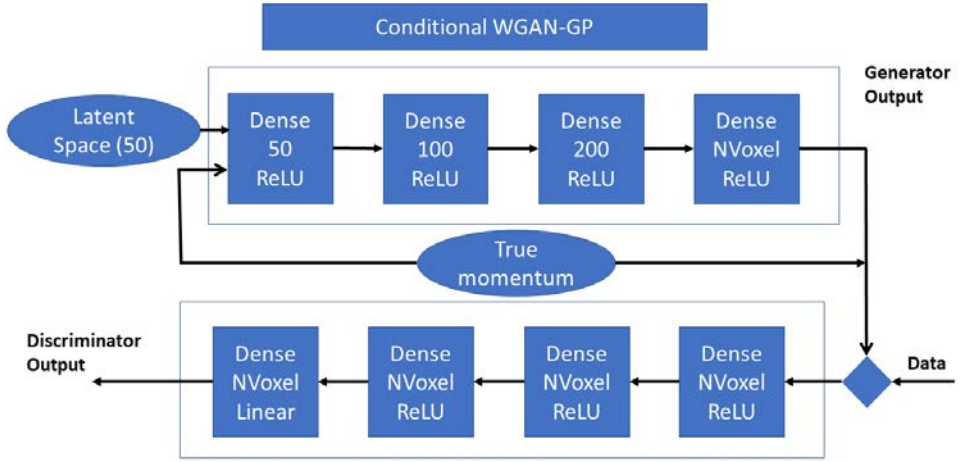


arXiv:2311.17175



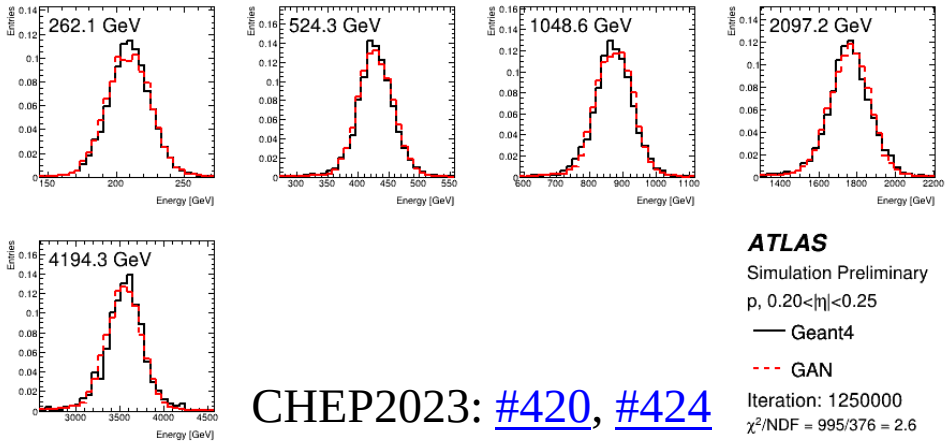


Generative Models for ATLAS Simulation



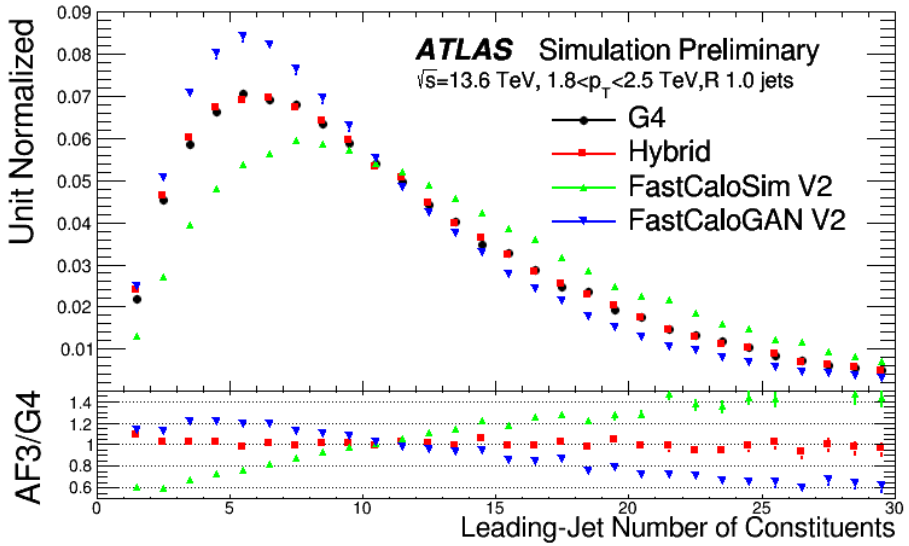
- FastCaloGAN architecture: Wasserstein loss prevents mode collapse
- Separate GANs trained for 100 η slices and for each particle type: γ, e, $\pi^{\pm}$, p → 600 total
  - Hyperparameters optimized for each particle
  - ~100 V100 GPU-days for final training
- Irregular geometry voxelized for training
- Incorporated in AtlFast3 along with FullSim and FastSim modules (depending on particle type, etc.)

- Good agreement for protons (new!)



CHEP2023: #420, #424

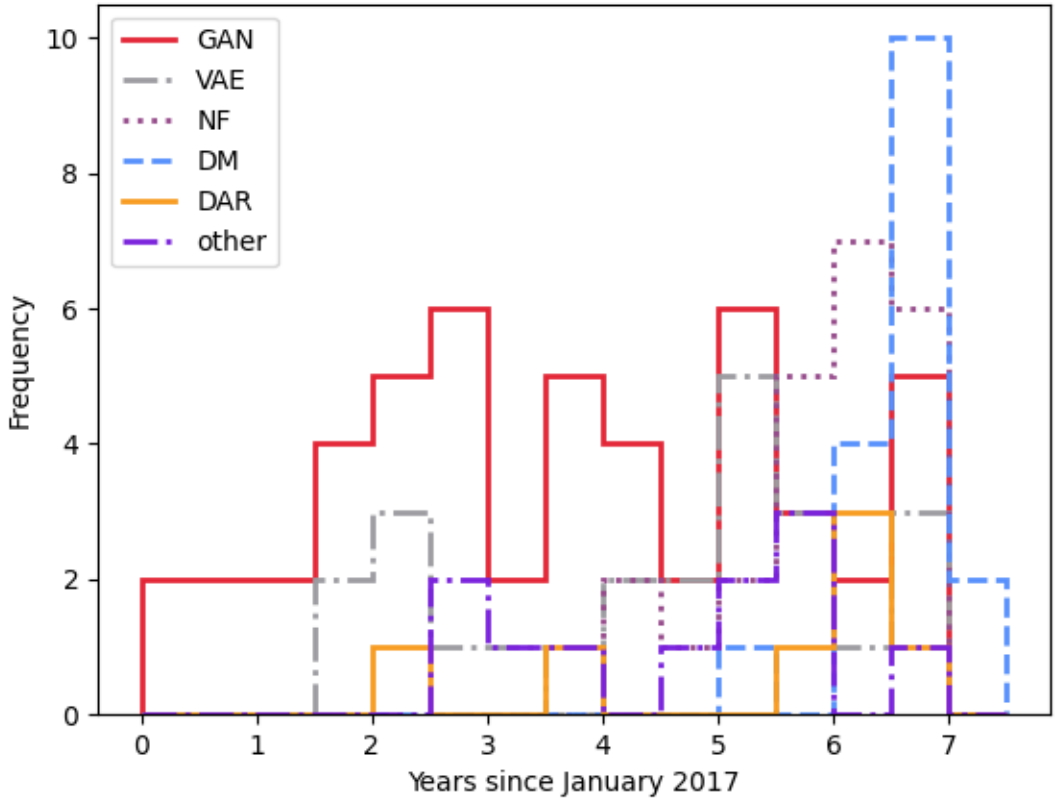
- Hybrid approach improves modeling of high-level quantities



7 Years of ML4Sim

Simulation

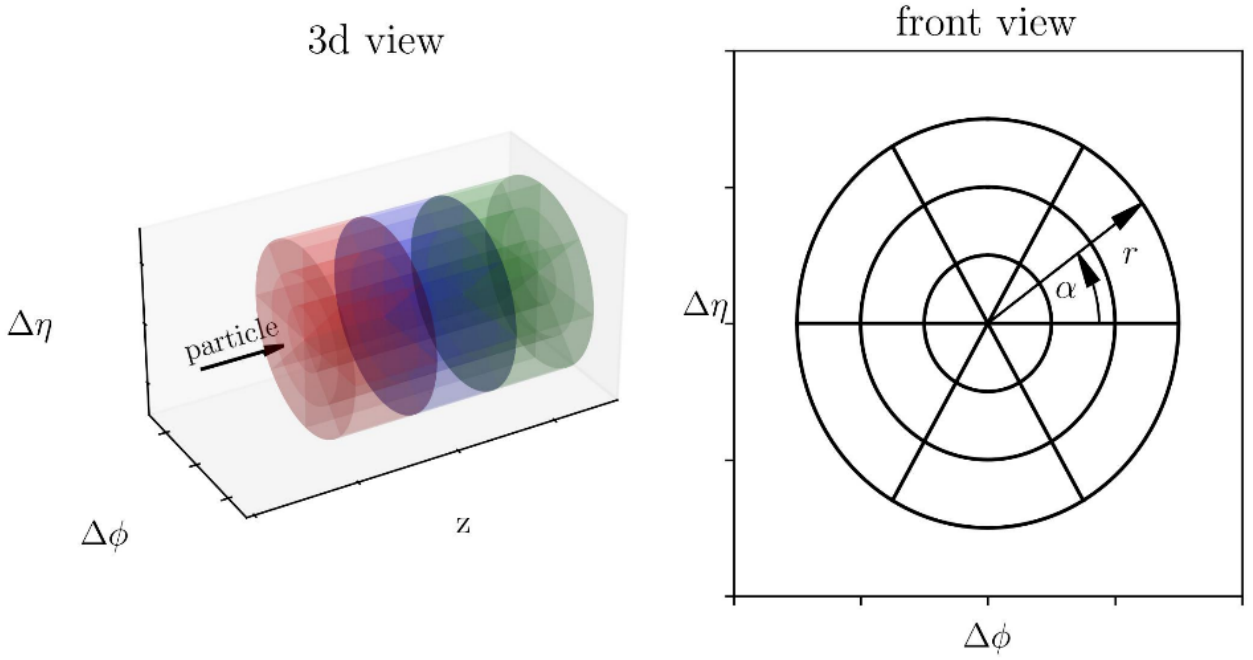
- From my database of 100+ ML4Sim-related papers
- Normalizing flows and diffusion models supplanting traditional GANs and VAEs
- Almost exponential takeoff for diffusion models
  - Following industry dominance in image generation Stable Diffusion, DALL·E, Midjourney, etc.
- Some growing interest in autoregressive models
  - Perhaps motivated by success in industry (GPT)
- Common datasets and metrics: big step forward to compare different approaches



"Other" = non-generative models (FCNs, CNNs, GNNs), typically regression-based approaches

CaloChallenge

Simulation



- CaloChallenge: first competition for generative ML for detector simulation
- Three public datasets provided:
  1. Low granularity, irregular geometry (based on ATLAS calorimeter), photon & pion showers
  2. Medium granularity, silicon-tungsten sampling calorimeter, electron showers
  3. High granularity, otherwise same as #2

- Common datasets are crucial to compare different generative methods
  - Using metrics discussed on next slide
- Many new methods developed for the challenge
  - Preliminary comparisons will be shown

Metrics

Simulation

- Speed only matters if needed accuracy is achieved
  - Wrong answers can be obtained infinitely fast
- 1D histograms:
  - e.g. separation power $S(g,h) = \frac{1}{2}\sum \frac{(g-h)^2}{(g+h)}$
  - Can miss high-dimensional correlations
- Best category: **integral probability metrics**

$$D_{\mathcal{F}}(p_{\text{real}}, p_{\text{gen}}) = \sup_{f \in \mathcal{F}} |\mathbb{E}_{\mathbf{x}\sim p_{\text{real}}} f(\mathbf{x}) - \mathbb{E}_{\mathbf{y}\sim p_{\text{gen}}} f(\mathbf{y})|$$

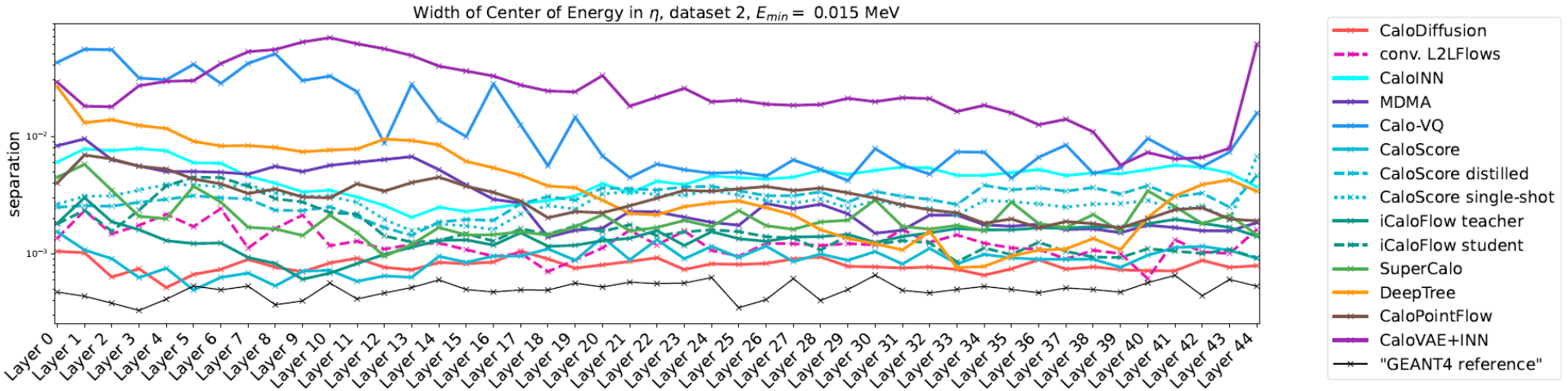
  - *Wasserstein distance* W_1: $\mathcal{F}$ is set of all K-Lipschitz functions
    - Only works well in 1D, biased in high-D
  - *Maximum mean discrepancy* (MMD): $\mathcal{F}$ is unit ball in reproducing kernel Hilbert space
    - Depends on choice of kernel
  - *Fréchet distance*: W_2 distance between Gaussian fits to (high-D) feature space
    - Features can be hand-engineered or obtained from NN activations
- Another interesting category: *classifier scores*
  - Train NN to distinguish real vs. generated
  - AUC score: ranges from 0.5 to 1.0
  - Log-posterior probability in multiclass case
- *Fréchet Particle Distance* most clearly distinguishes between two similar approaches

	FPD $\times 10^3$	KPD $\times 10^3$	W_1^M $\times 10^3$
Truth	0.08 ± 0.03	-0.006 ± 0.005	0.28 ± 0.05
MPGAN	$\mathbf{0.30 \pm 0.06}$	$\mathbf{-0.001 \pm 0.004}$	$\mathbf{0.54 \pm 0.06}$
GAPT	0.66 ± 0.09	0.001 ± 0.005	0.56 ± 0.08

arXiv:2211.10295

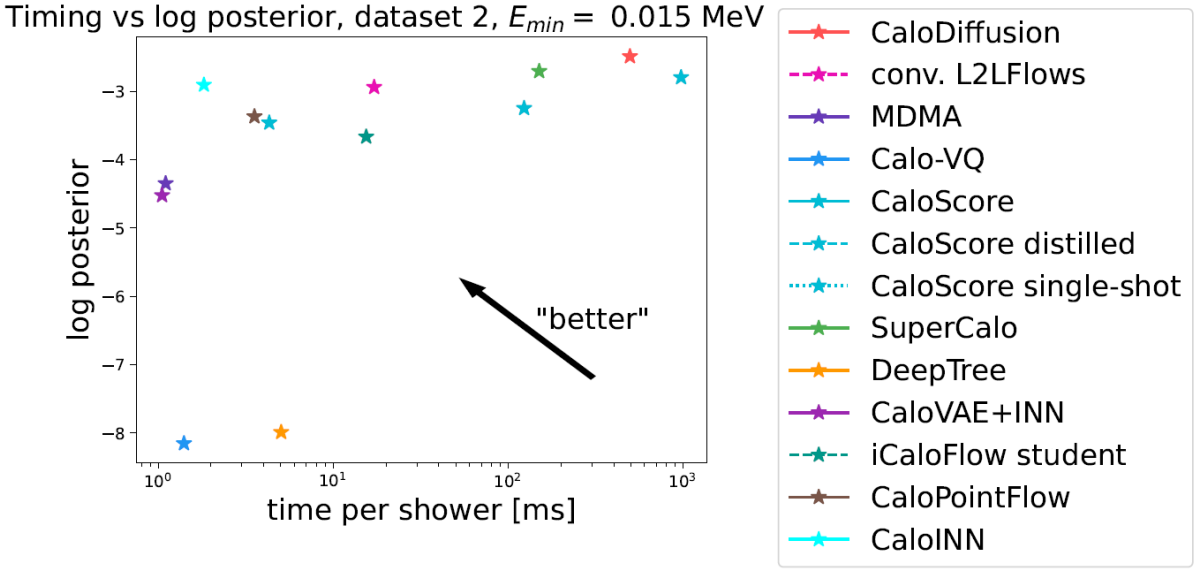
CaloChallenge Results

Simulation



- Diffusion models and normalizing flows tend to have best performance
- However, diffusion models especially tend to be slower in inference
  - Iterative process – multiple steps required to get highest accuracy

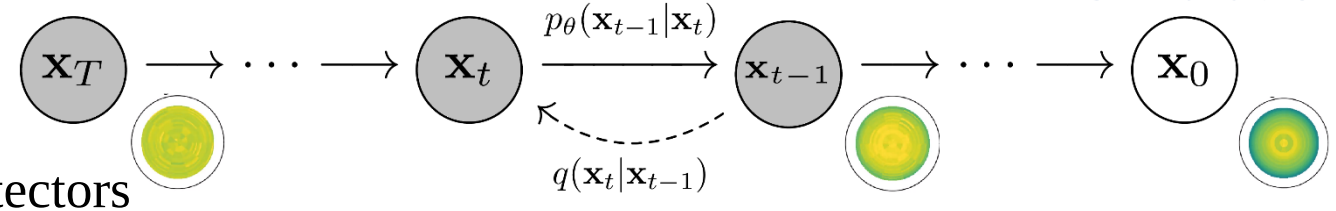
C. Krause

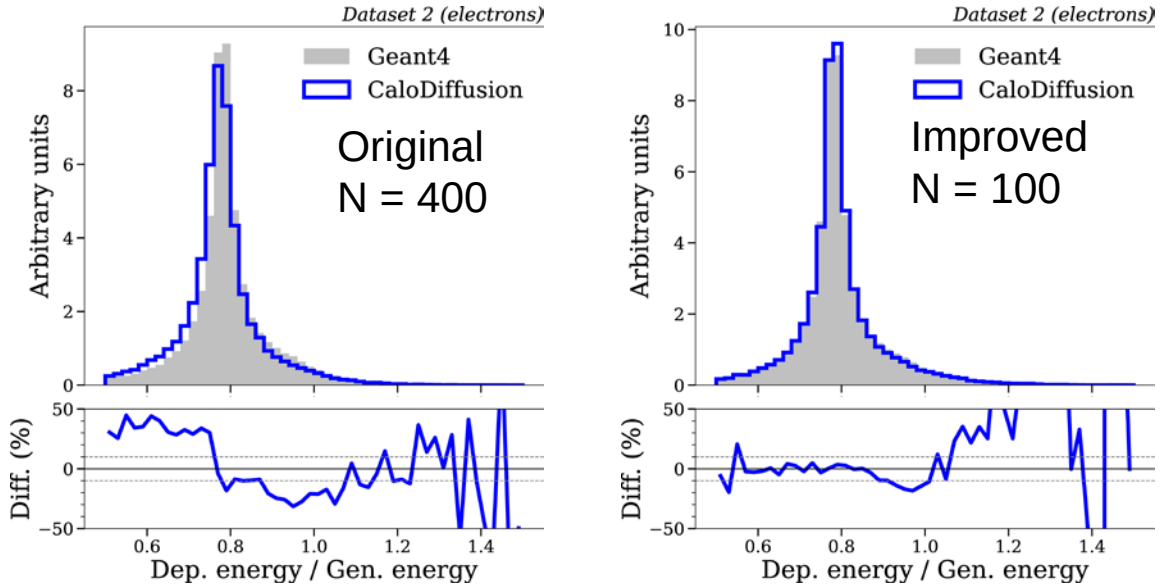


CaloDiffusion

Simulation

- Current state-of-the-art model: denoising w/ convolutional U-net architecture
  - Various geometric adaptations:
    - Conditional cylindrical convolutions
    - Geometry latent mapping for irregular detectors
    - Attention layers for long-range correlations in *z*
- Improvement from original: LayerDiffusion to predict total energy per layer → 4× speedup & better quality
  - More speedups in [arXiv:2401.13162]





- Comparison to other SOTA models:
  - Best classifier AUC scores
  - Low distance values compared to Geant4

Classifier AUC (low / high)

Dataset	CaloDiffusion	CaloFlow	CaloScore v2
1 (photons)	**0.62** / 0.62	0.70 / **0.55**	0.76 / 0.59
1 (pions)	**0.65** / **0.65**	0.78 / 0.70	- / -
2 (electrons)	**0.56** / **0.56**	0.80 / 0.80	0.60 / 0.62
3 (electrons)	**0.56** / **0.57**	0.91 / 0.95	0.67 / 0.85

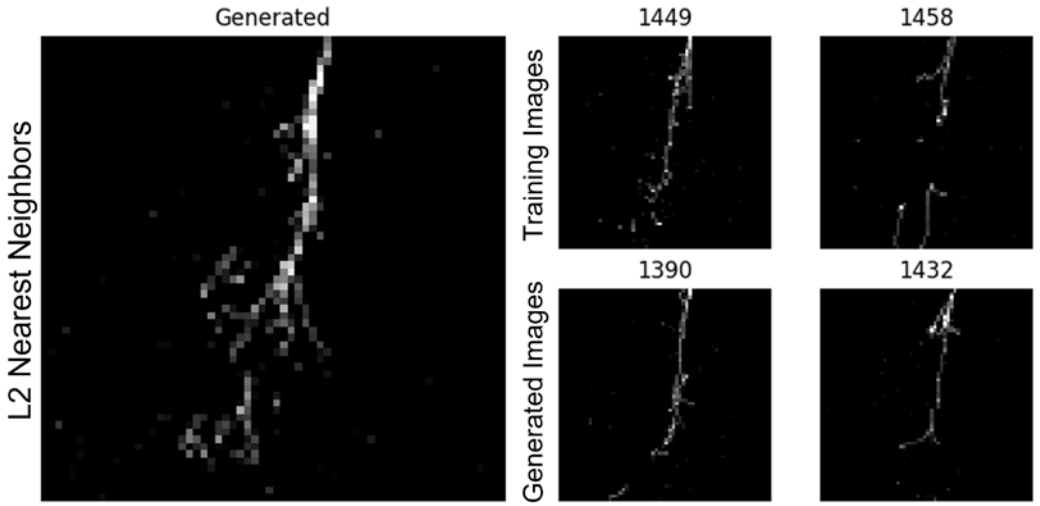
Dataset	FPD†	KPD
1 (photons)	0.014(1)	0.004(1)
1 (pions)	0.029(1)	0.004(1)
2 (electrons)	0.043(2)	0.0001(2)
3 (electrons)	0.031(2)	0.0001(1)

[arXiv:2308.03876]

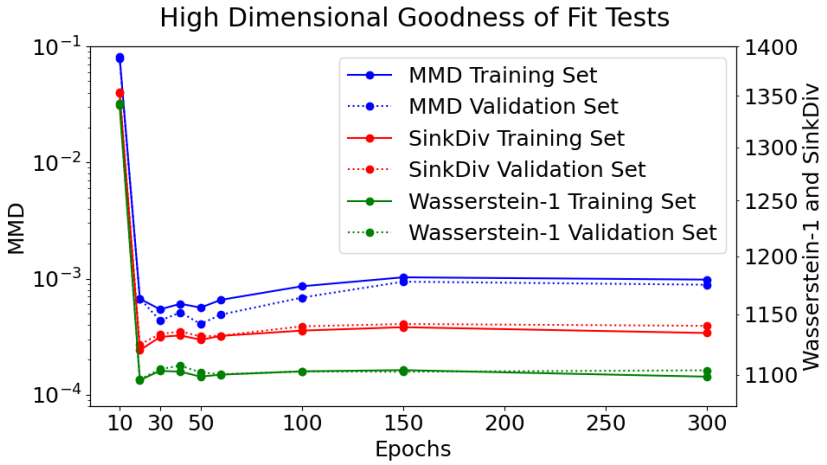
Diffusion for Liquid Argon TPCs

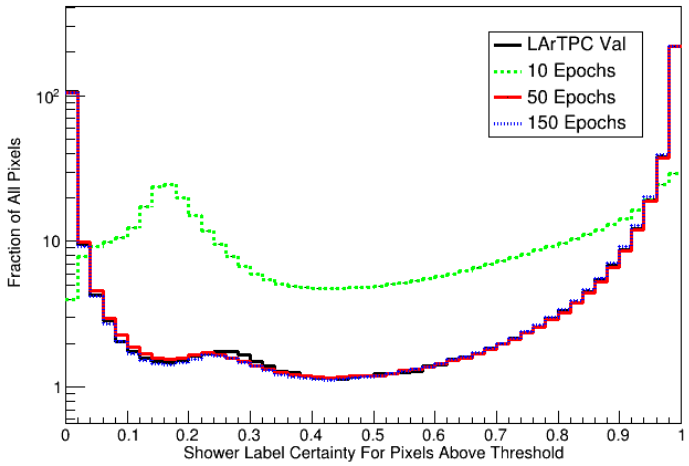
Simulation

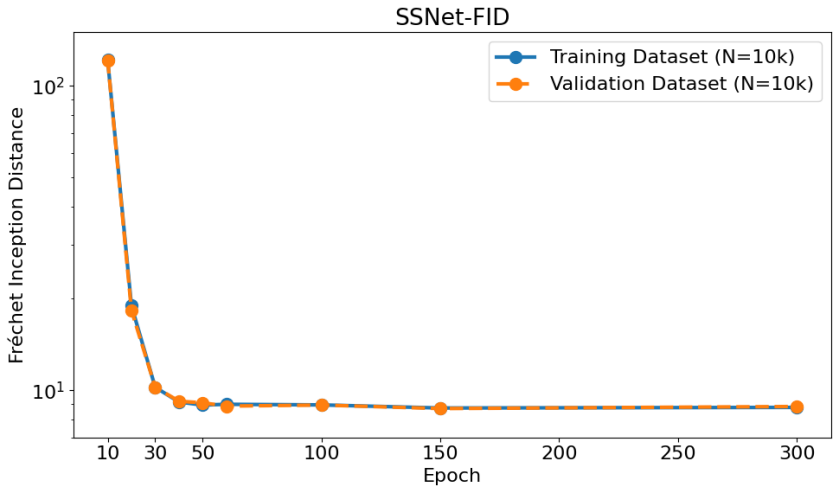
- Diffusion models can also simulate ionization deposits from charged tracks in LAr TPC detectors
  - Here, score-based rather than denoising model is used
- Both visual and quantitative comparisons
  - Various distance metrics, SSNet scores, Fréchet inception distance (from SSNet activations)
- Superior to previous attempts (VAE)



arXiv:2307.13687



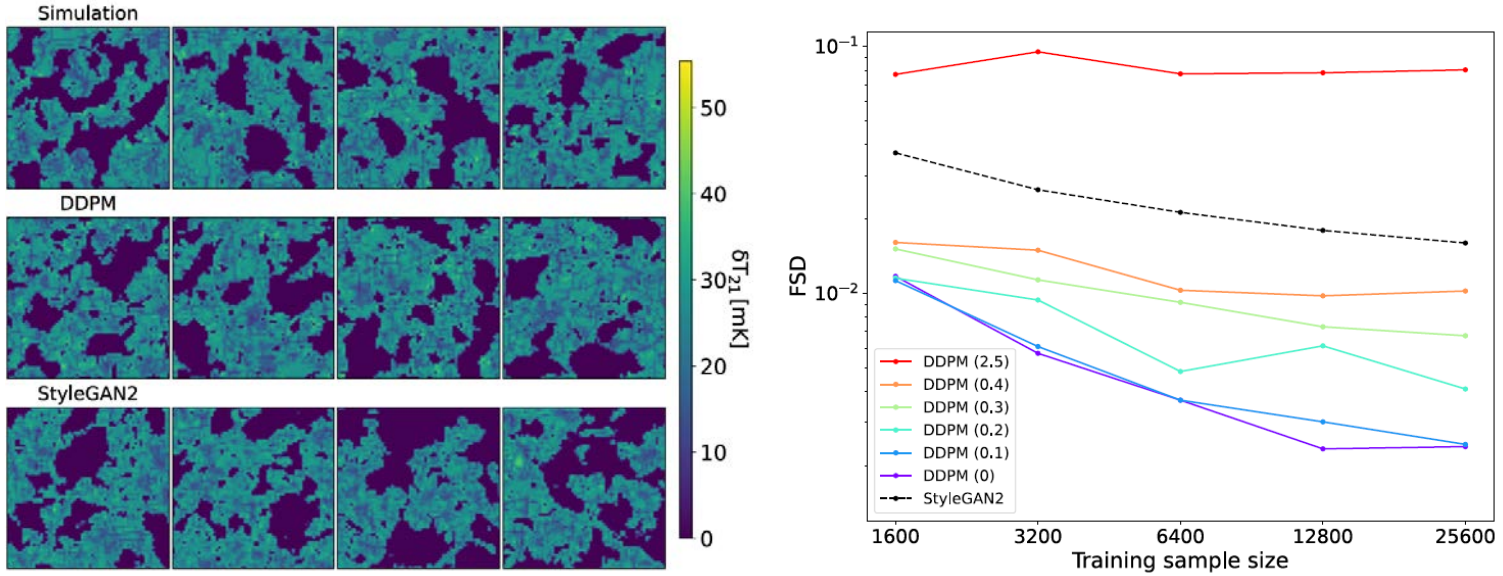




Diffusion for Astrophysical Images

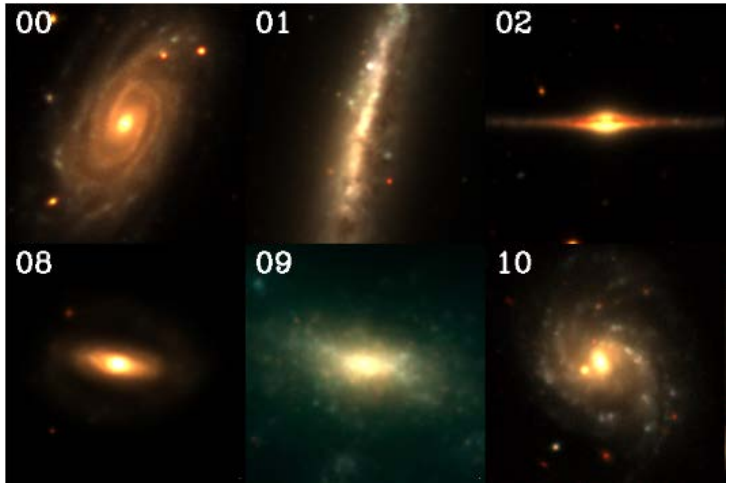
Simulation

- Diffusion models can simulate various astrophysical phenomena
  - Denoising DM for CMB maps (21 cm brightness temperature)
- Quantified using Fréchet scattering distance (from coefficients)
  - Substantial improvement over GANs
  - ~100× slower than GANs, but GPU inference still ~5× faster than traditional CPU-based simulation

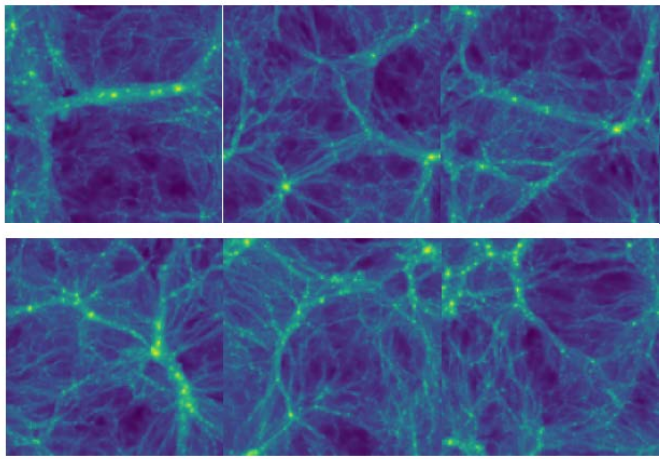


arXiv:2307.09568

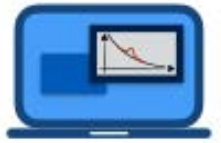
- Also applied to:
  - Galaxy images (arXiv:2111.01713)



  - Dark matter maps (arXiv:2211.12444)

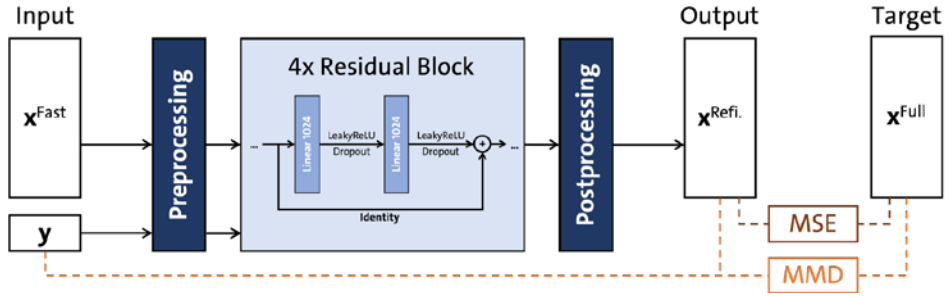


High-Level Refinement

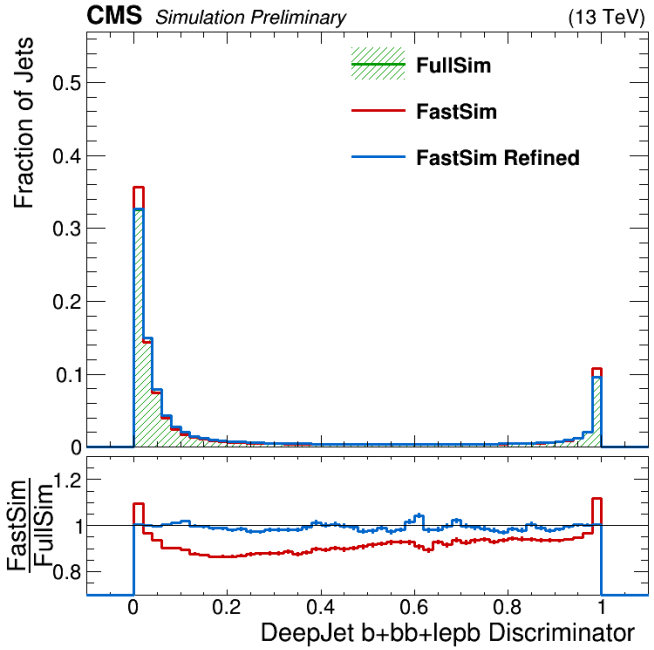


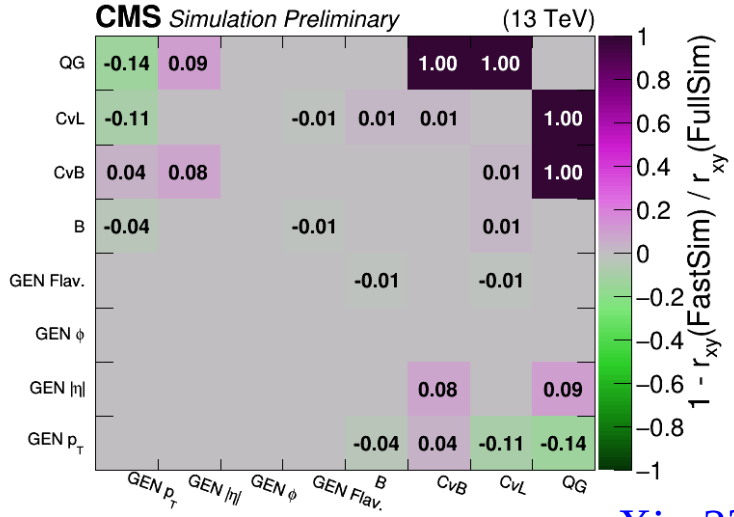
Analysis

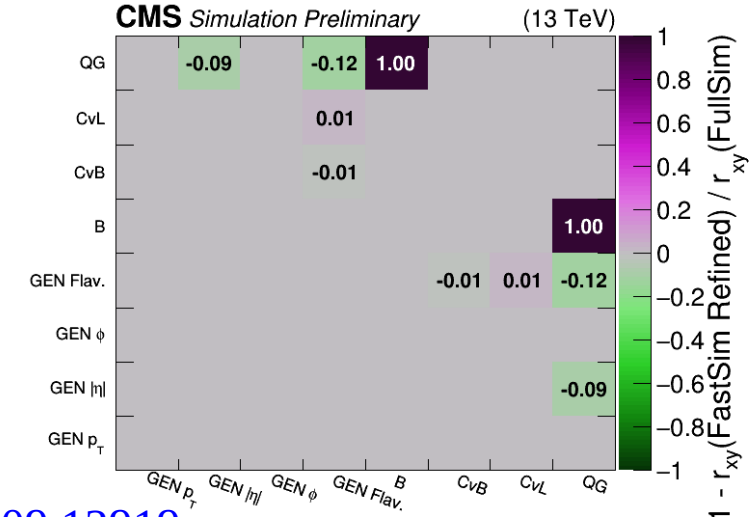
- Alternate approach: ML adjusts high-level quantities from existing CMS FastSim to match FullSim
  - o Replaces coarse, manual correction factors
- Loss functions: ensemble & object-by-object comparisons
- Improves metrics, 1D distributions, correlations
- Generalizes to other processes; now being extended to more variables for Run 3 deployment



FullSim vs.	FPD $\times 10^3$	KPD $\times 10^3$
FastSim	0.801 ± 0.046	1.07 ± 0.58
FastSim Refined	0.071 ± 0.025	0.083 ± 0.418
FullSim	0.061 ± 0.029	-0.024 ± 0.250

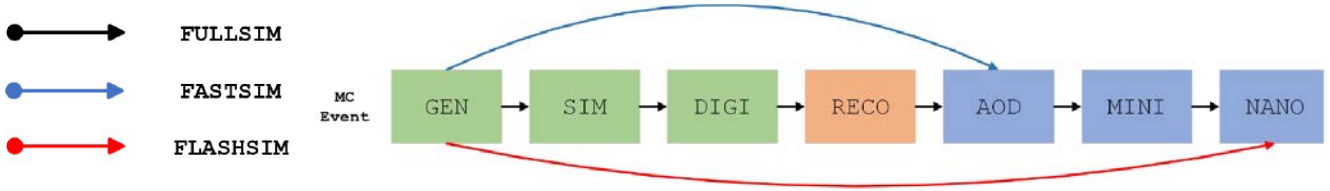






arXiv:2309.12919

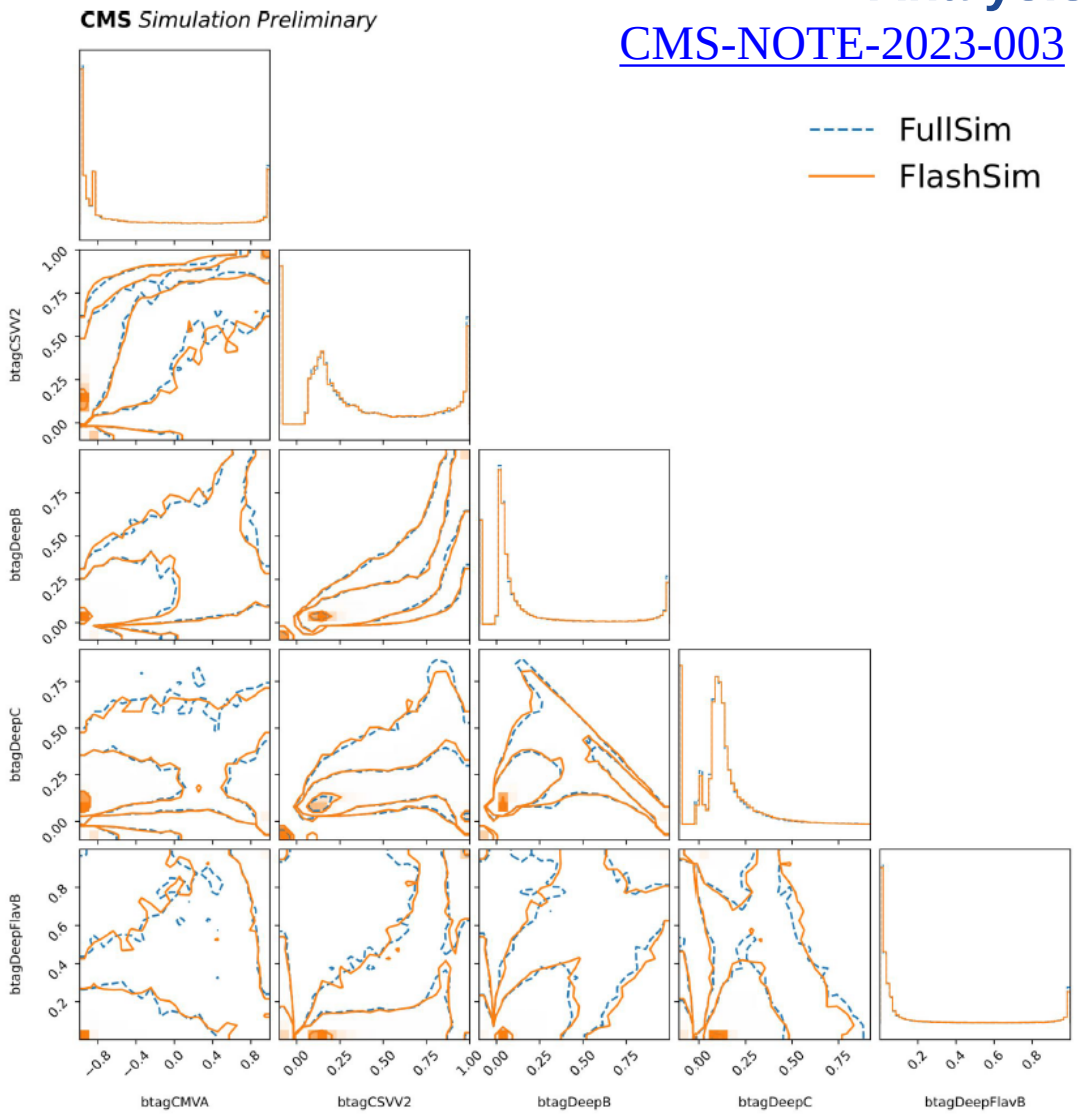
End-to-end: FlashSim



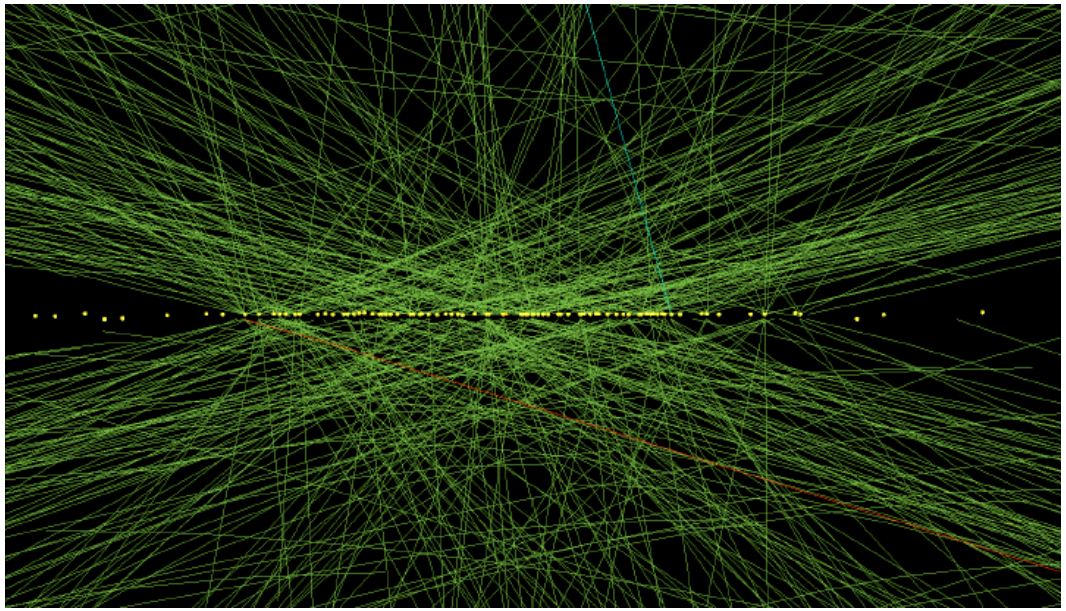
- Normalizing flow to predict high-level analysis quantities from generator-level information
- Reproduces correlations even in ML b-tagging algorithm scores
- Currently covers: jets (real & fake), muons, electrons
- Very promising solution for end-stage analyses
  - Effectively infinite event sample
    → minimize statistical fluctuations
- Complementary w/ simulation step solutions
  - Need to develop calibrations, algorithms, etc. to produce training data for FlashSim
    - These tend to vary more rapidly than geometry

Analysis

[CMS-NOTE-2023-003]



Pileup: An Overlooked Case



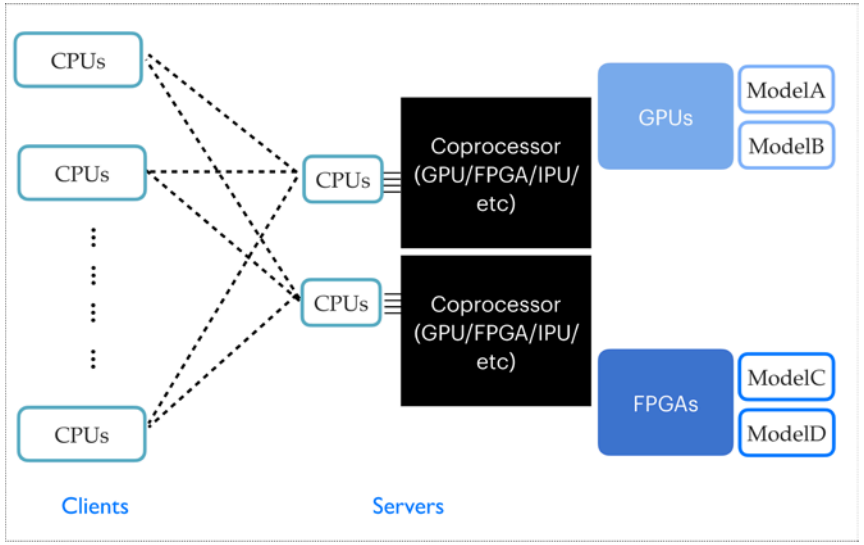
- "Classical" mixing: overlay n_{PU} *distinct* simulated minimum bias events *per bunch crossing* on top of signal event → massively I/O intensive
- "Premixing": perform overlay in advance, save hits after aggregation (digitized format)
  - Leads to O(PB) samples that have to be served throughout the grid with very high availability
  - Better than classical mixing, but still disk- and network-intensive

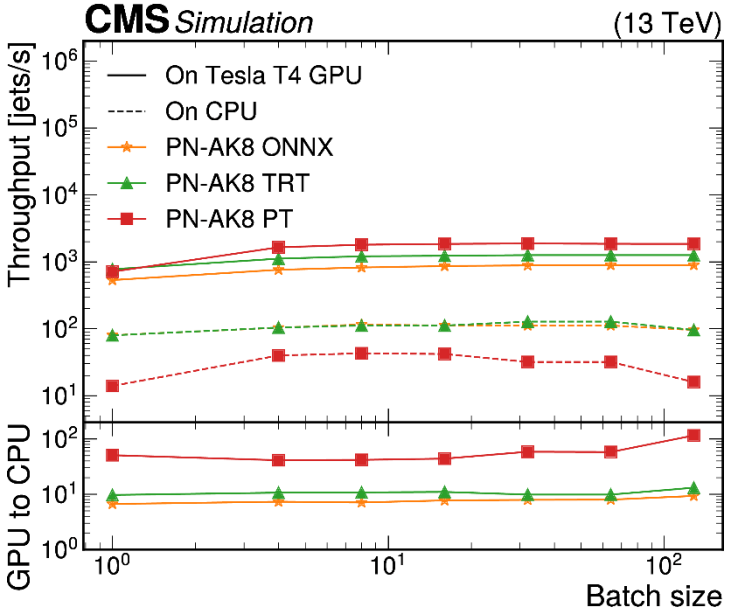
Digitization

- Viewed as a solved problem… but substantial room for improvement
  - Generative ML could compress O(PB) samples into O(MB) model + random number generator & conditioning info → *completely eliminate* premixing resource usage (in exchange for training)
- Straightforward to repurpose detector simulation surrogates, but also possible improvements here
  - Train on data and realize long-awaited data mixing?
- Similar principles apply to e.g. beam-induced backgrounds, dust overlays, etc.

Computing for ML

- ML algorithms use a restricted set of operations (mostly matrix multiplications)
  - Natural and easy to accelerate on specialized coprocessors
- *Most flexible* approach: inference as a service
  - Abstract away specific computing elements: client makes request, server delivers
  - Example: ParticleNet 10–100× faster on GPU vs. CPU
    - Algorithm latency becomes essentially *invisible* with asynchronous calls in offline processing
    - Can batch *across events* for optimal GPU utilization → maximize throughput
- Demonstrated for CMS, protoDUNE, LIGO, analysis facilities
  - Use CPUs, GPUs, FPGAs, TPUs, IPUs… with zero code changes!
  - Optimally exploit new GPU-based High Performance Computing (HPC) facilities





Conclusion

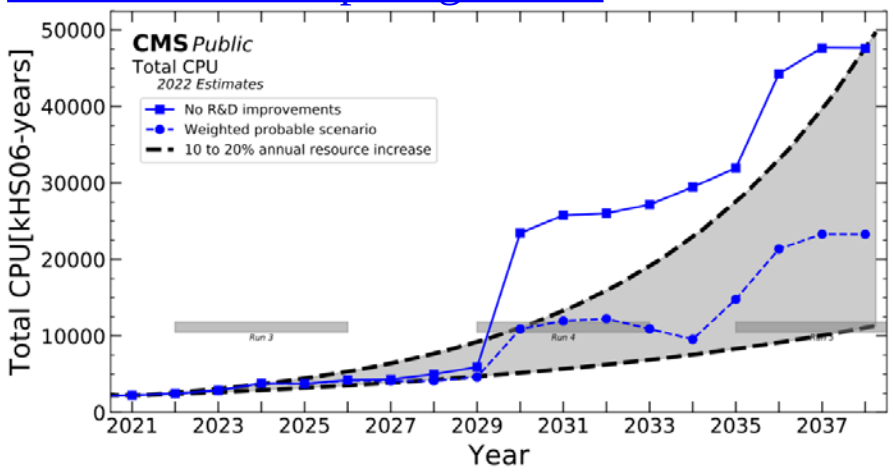
- Growing usage of AI/ML methods for event generation and simulation
  - Both generative models and non-generative classification/regression techniques are useful
- Increasing focus on resolving *practical problems*: improve both *accuracy* and *computing time*
  - Implementing in common or experiment software frameworks
  - Using ML at production scale – beyond proof of concept
- Applications throughout HEP
  - Primarily investigated for collider physics so far
  - Neutrino and astrophysics starting to see more adoption
- Diffusion models particularly powerful
  - Techniques like flow matching poised to unify normalizing flows and diffusion models
- Many more novel applications than could be discussed here
  - SIM reviews: arXiv:2203.08806, arXiv:2312.09597
  - GEN reviews: arXiv:2202.05991, arXiv:2203.07460
  - Overall: HEPML-LivingReview

Background generated by SDXL 1.0 w/ prompt: “A GEANT4 simulation of a pion shower with energy 100 GeV in the Compact Muon Solenoid High Granularity Calorimeter at the CERN Large Hadron Collider, a particle physics experiment”

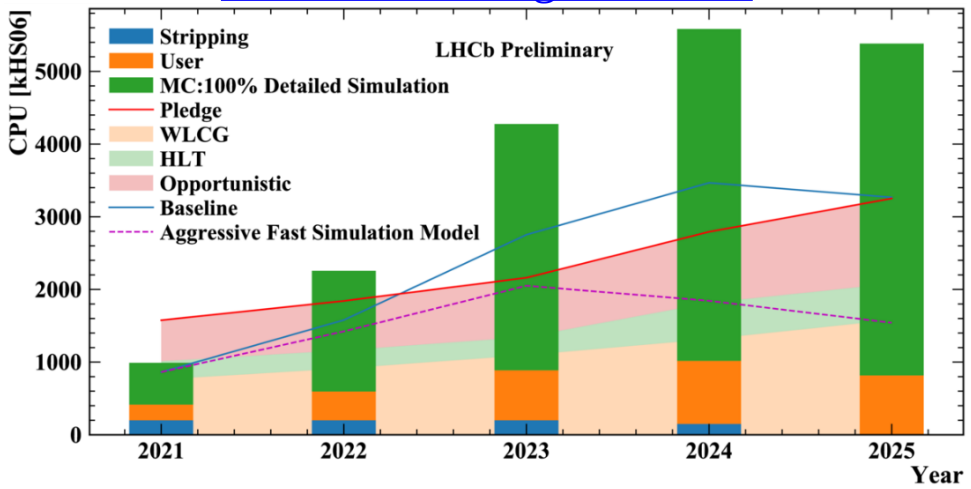
Backup

Projections

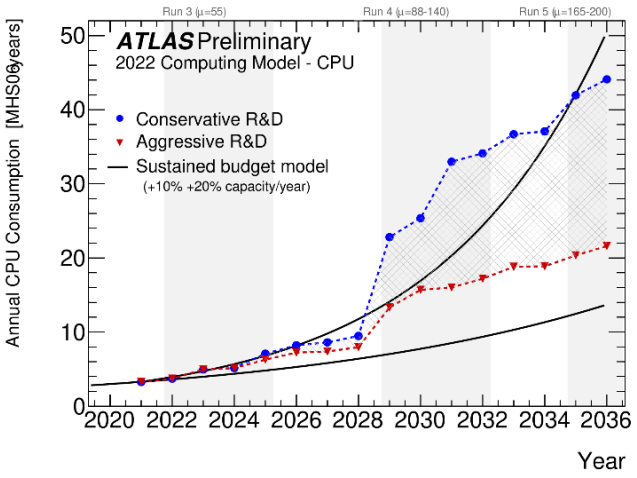
CMSOfflineComputingResults

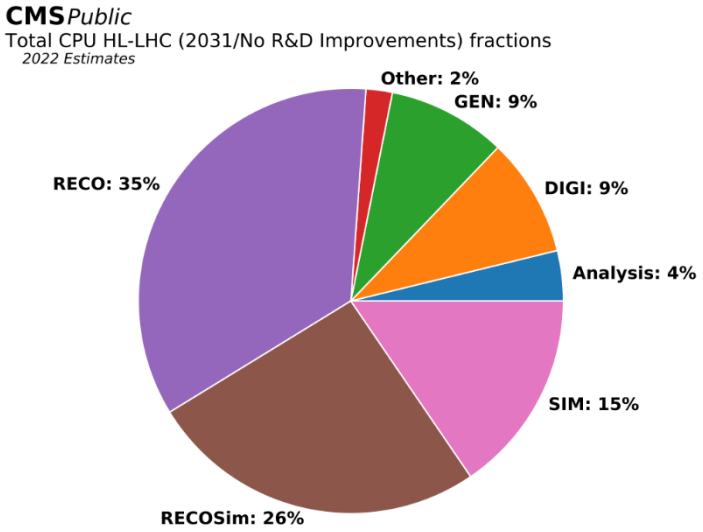


LHCb CPU Usage Forecast

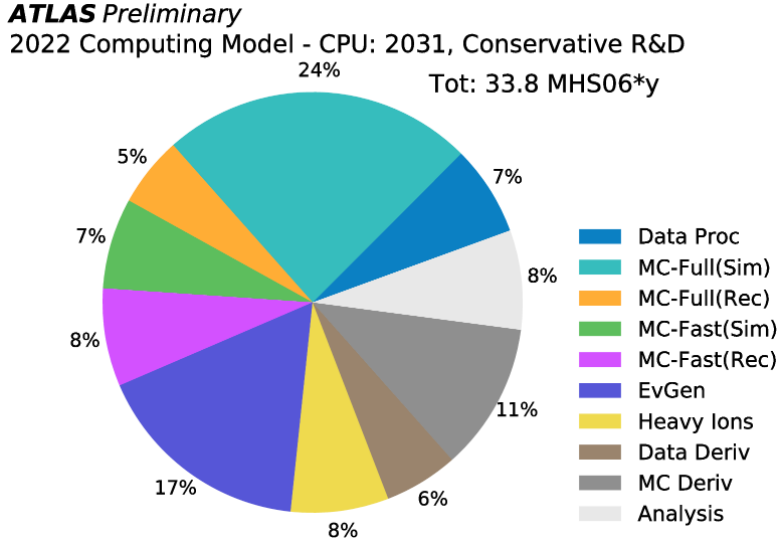


CERN-LHCC-2022-005

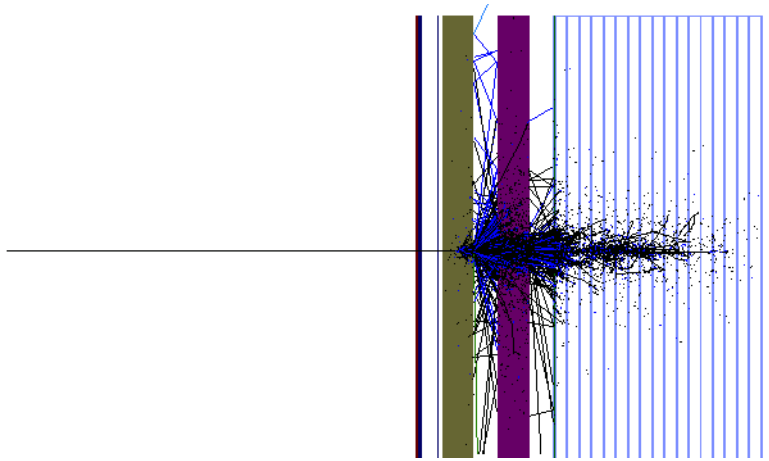




- Run 2: (full) simulation used ~40% (plurality) of grid computing resources for CMS & ATLAS [arXiv:1803.04165]
  - 70% for LHCb! [LHCb-PUB-2022-010]
- Run 4+: limit to ~10–20%, while simulating:
  - Complex detector upgrades
    - e.g. CMS High Granularity Calorimeter
  - More precise physics models
  - More events to reduce statistical uncertainty



Simulation Landscape

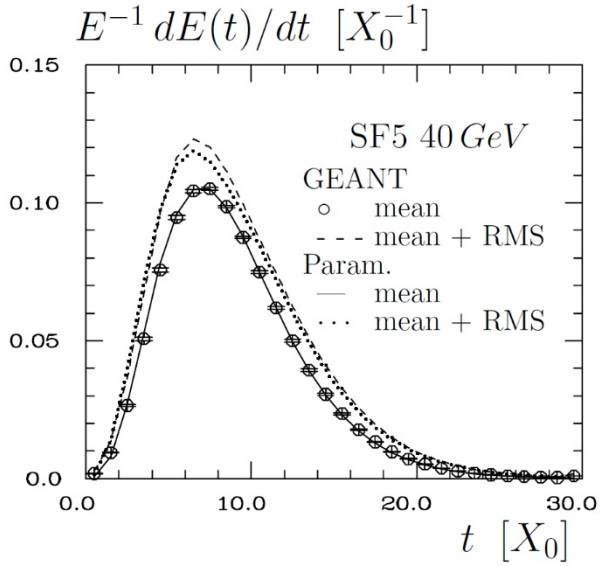


“FullSim”

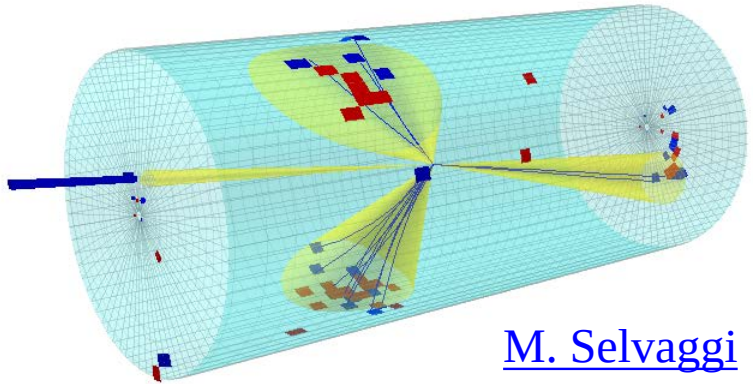
- Common software framework (i.e. Geant4)
  - Experiments can provide additional code via user actions
- Explicit modeling of detector geometry, materials, interactions w/ particles

“FastSim”

- Usually experiment-specific framework
- Implement approximations: analytical shower shapes (e.g. GFLASH), truth-assisted track reconstruction, etc.



arXiv:hep-ex/0001020



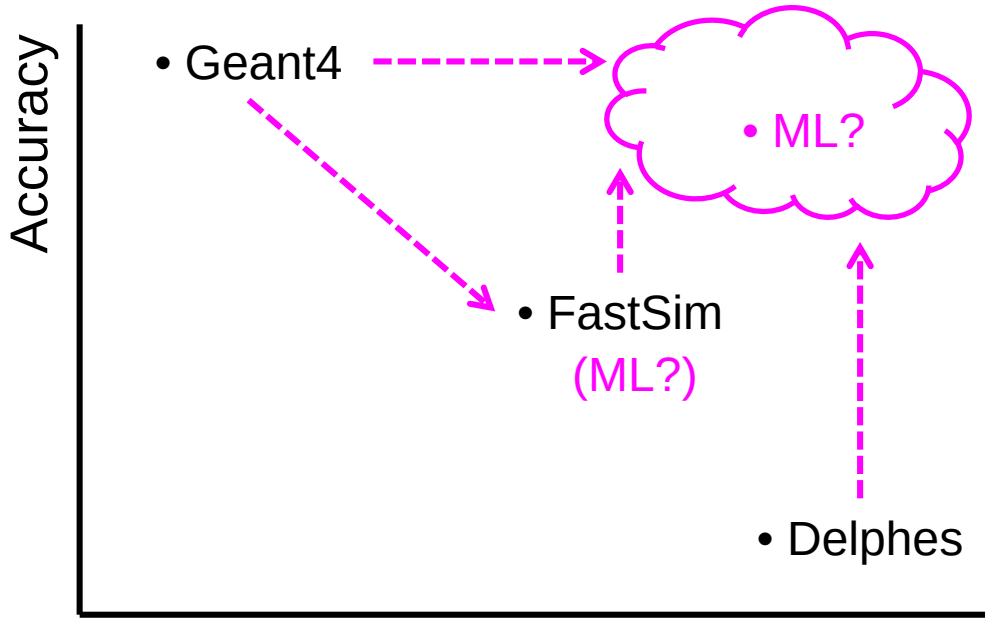
M. Selvaggi

Delphes

- Ultra-fast parametric simulation
- Used for phenomenological studies, future projections, etc.

ML4Sim Landscape

- Options to use ML for sim:
  1. Replace or augment (part or all of) Geant4
  2. Replace or augment (part or all of) FastSim
- Goals:
  1. Increase speed while preserving accuracy
  2. Preserve speed while increasing accuracy
- ML can also create faster, but less accurate simulation
  - à la existing classical FastSim
    - then augment w/ more ML to improve accuracy
- Another option: replace entire chain (“end-to-end”)
  - Complements other cases



arXiv:2203.08806

Constrained Optimization

- *General principle*: you can't optimize for two things at once
  - Instead, optimize for one thing with *constraints* on others (Lagrange)
- Multiple loss terms are one approach to encode domain knowledge

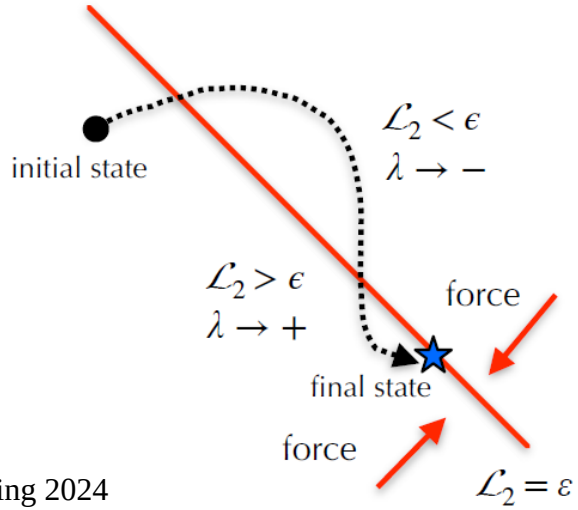
☠ $\mathcal{L} \to \mathcal{L}_1 + \lambda\mathcal{L}_2 + \cdots$; set λ by trial and error → *objectively suboptimal*

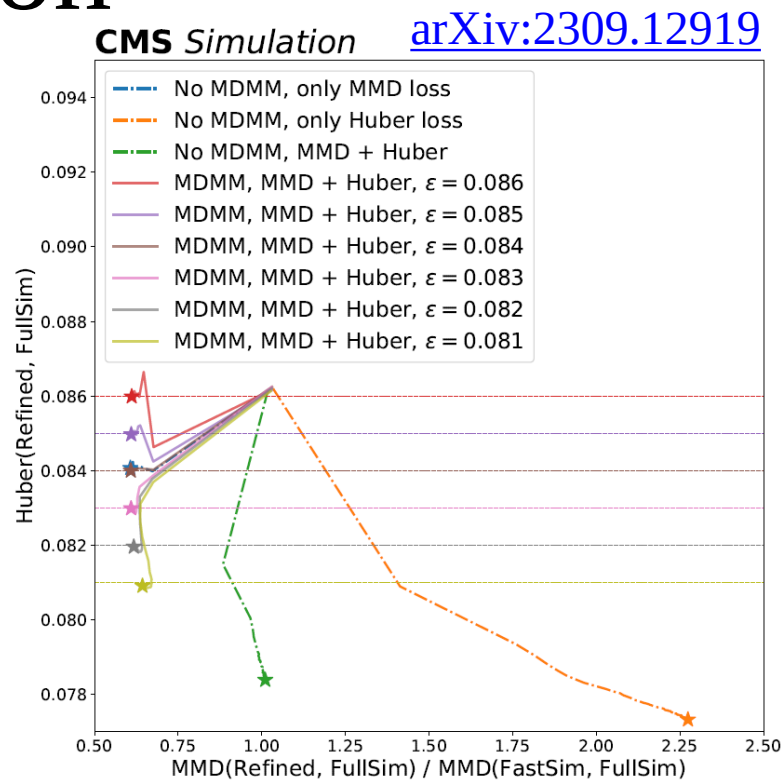
➢ modified differential method of multipliers (mdmm): [paper, blog, code]

learnable hyperparameter (convergence rate)

$$\mathcal{L} \to \mathcal{L}_1 - \lambda(\varepsilon - \mathcal{L}_2) + \delta(\varepsilon - \mathcal{L}_2)^2$$

gradient *ascent* constraint damping to ensure convergence



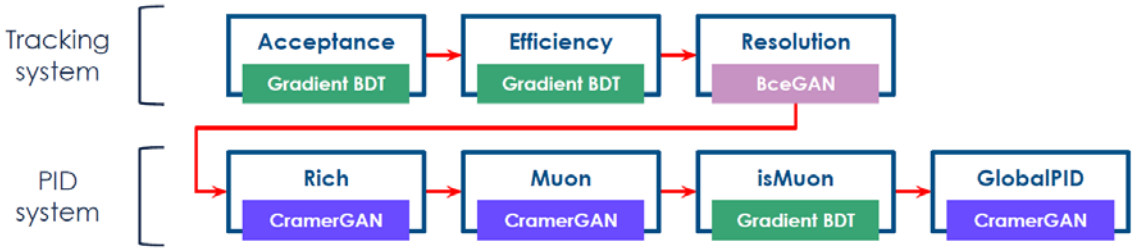


arXiv:2309.12919

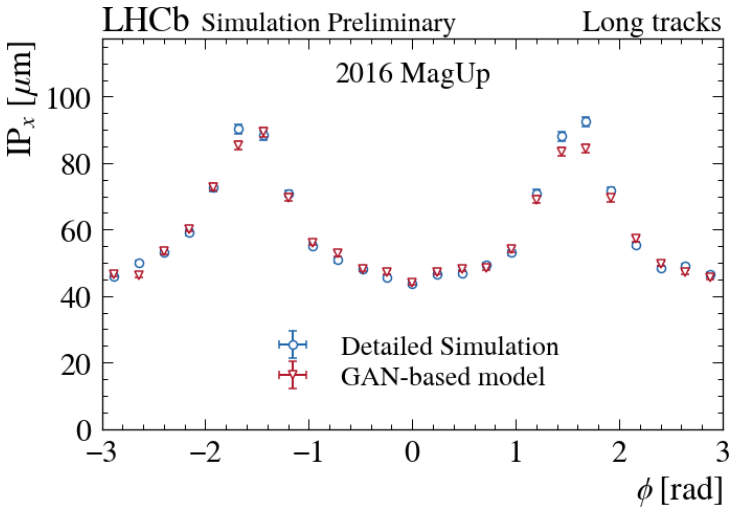
- First known usage in HEP: balance per-event and ensemble losses for ML-based refinement of classical FastSim
  - Minimize per-event: bad ensemble value
  - Minimize ensemble: per-event still good!

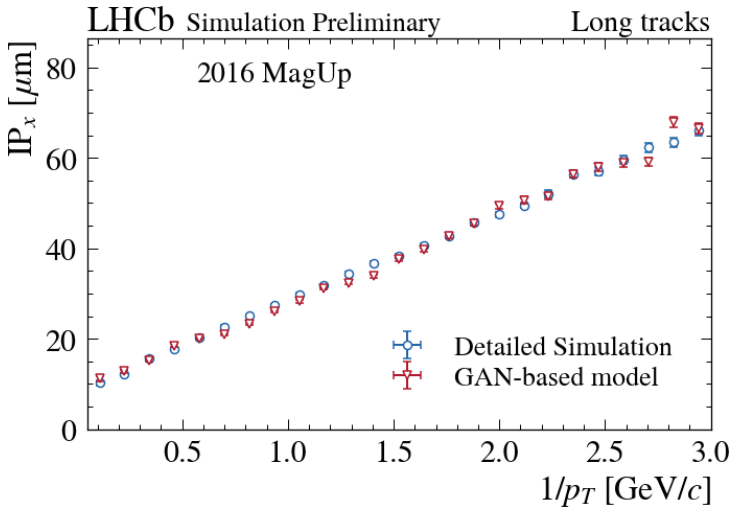
➢ Find Pareto front (concave or convex) and pick tradeoff

Generative Models at Colliders: LHCb

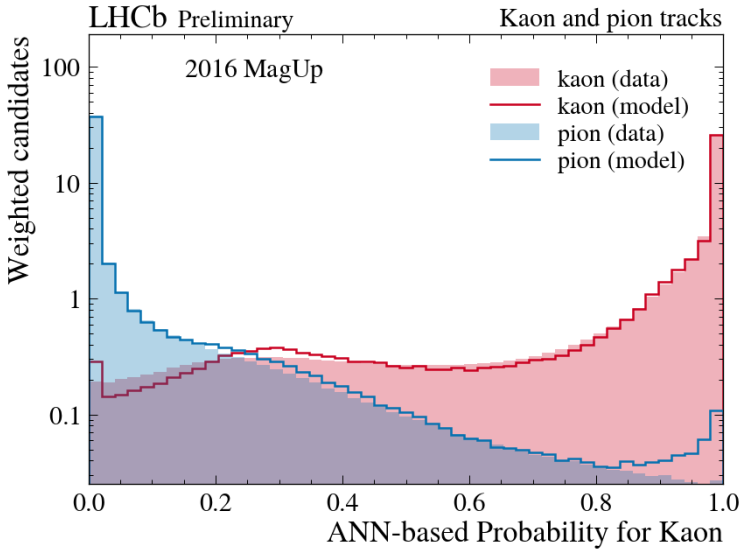


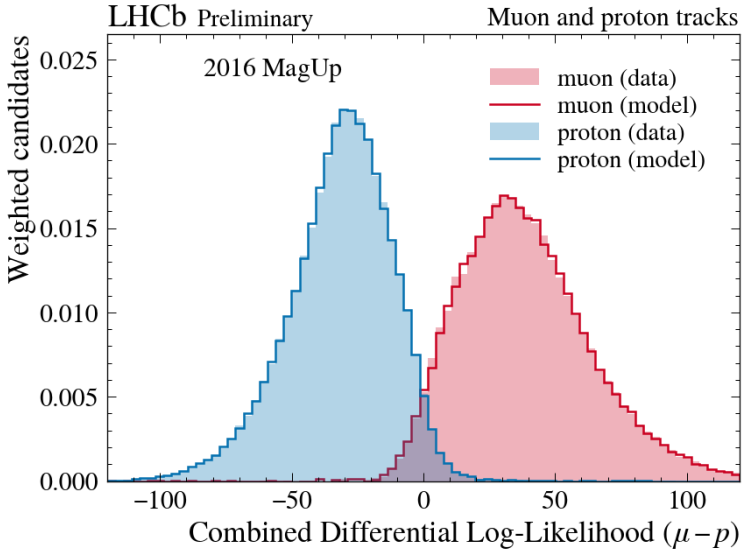
- "Stacked GAN" approach to parameterize different detector aspects
  - Cramér distance related to W_1
- Tracking resolution: well reproduced in p_T & φ





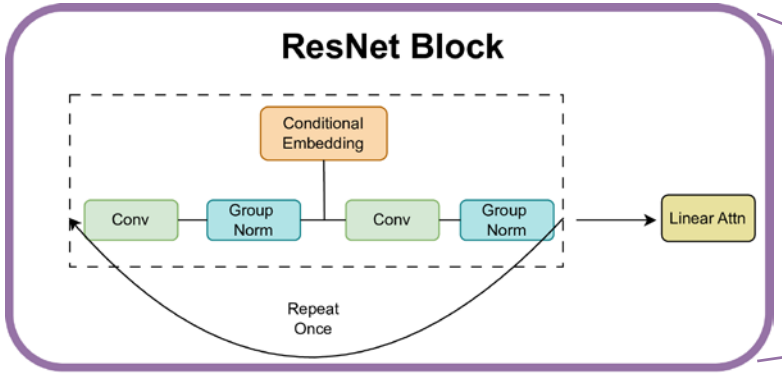
- Global PID variables also well reproduced:
  - Top: $K^{\pm}$ vs. $\pi^{\pm}$
  - Bottom: μ vs. p

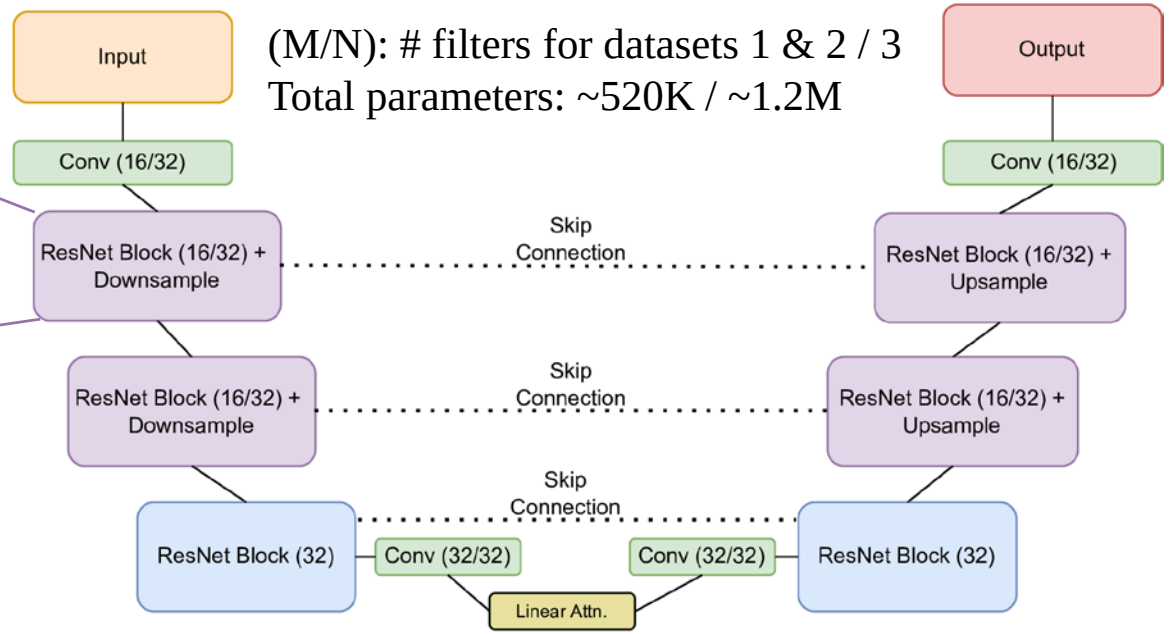




[LHCB-FIGURE-2022-004]

CaloDiffusion



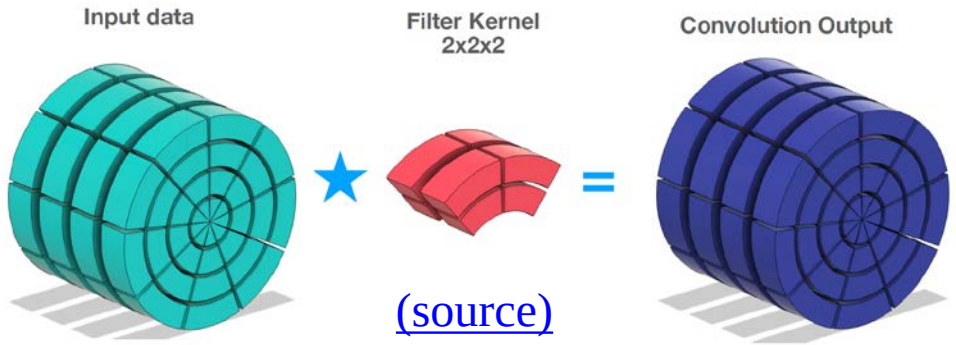


- Base architecture: U-net
  - Skip connections ensure no loss of information
- Linear self-attention layers applied to each convolutional ResNet block
  - Allows dimensionality reduction in *z* to handle longitudinal correlations in showers
- + numerous geometric innovations (next slide)
- Cosine noise schedule for training
- Stochastic sampling algorithm for generation

- Objectives:
  - Datasets 1 & 2: predict (normalized) noise
  - Dataset 3: predict weighted average of noise and denoised image
- Aim for highest achievable quality first
  - Then focus on improving speed
  - Wrong answers can be obtained infinitely fast

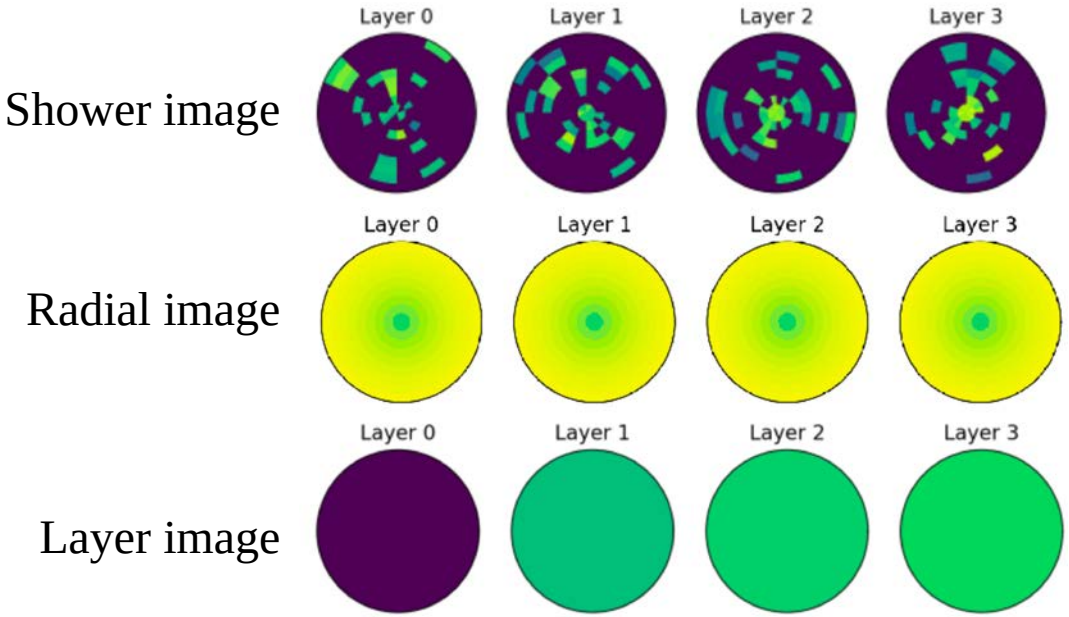
Geometric Innovations

- Particle showers are invariant & periodic in φ
  - Pad in φ so convolutions "wrap around"



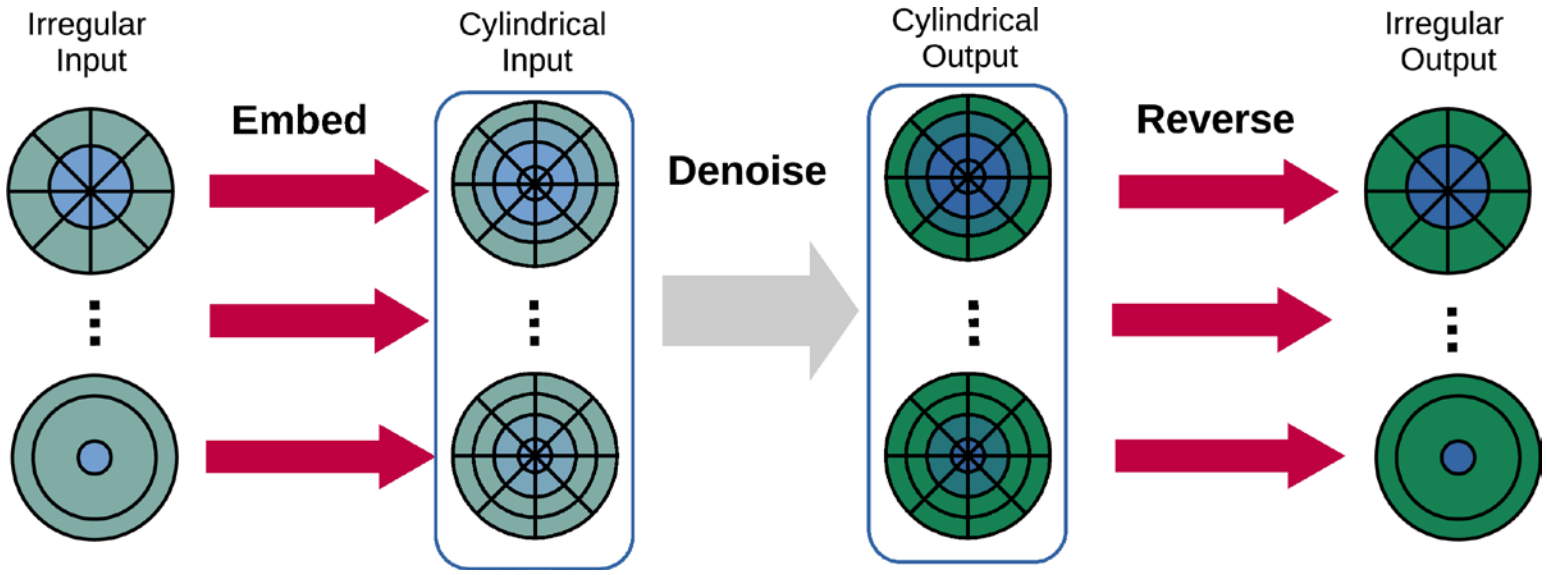
(source)

- Particle showers are *not* invariant in *r* or *z*
  - Provide *r* and *z* (layer) as extra per-pixel channels (input features)
  - Convolutions become *conditional*



➢ *Conditional cylindrical convolutions*
  - Handle inherent features of particle detector geometry, distinct from rectangular images

Geometry Latent Mapping: GLaM



- Dataset 1 has different radial/angular bins in each layer
  - Can't directly apply convolutions, which require regular neighbor structure
- Learn forward and reverse embeddings to and from a regular geometry
  - Simple matrices C (NxM) and D (MxN)
    - C initialized to split or merge cells based on overlap between original and embedded geometries
    - D initialized as Moore-Penrose pseudoinverse of C
- Inspired by "latent diffusion" approach
  - But not necessarily lower-dimensional representation; actually higher-dimensional here

Why Convolutions?

- Convolutions started the modern machine learning revolution (AlexNet, 2012)
  - *Spatial locality* and translational invariance
  - Shared weights → fewer parameters, *better scaling*
  - Highly *efficient* on GPUs: spatial locality implies memory locality
- Ideally suited for computer vision with rectangular images
  - Application to irregular geometries requires innovations
- Graph neural networks?
  - **Pro**: natural representation for irregular geometries
  - **Cons**: adjacency matrices consume substantial memory; operations less local/efficient; hard to generate arbitrary output (masking technique exists, but difficult to scale)
- Point clouds or transformers?
  - **Pro**: no adjacency matrix consuming memory
  - **Con**: discards useful geometric information, which then must be learned from (often sparse) inputs

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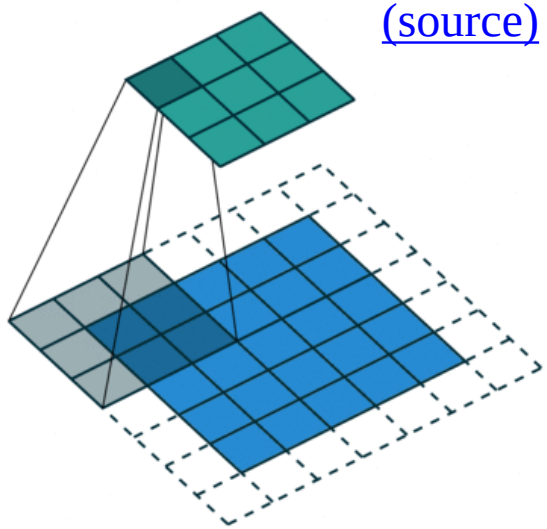
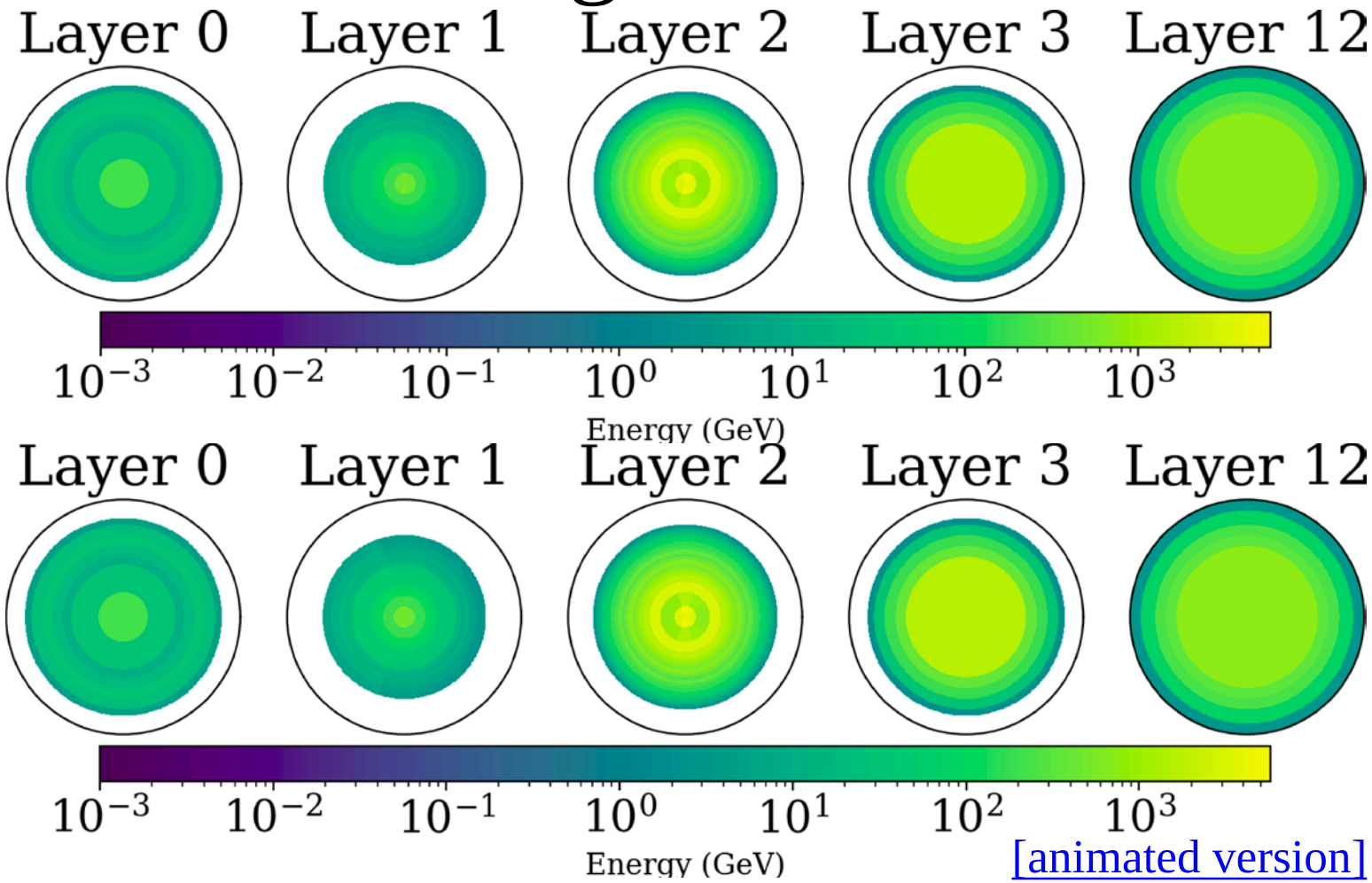


➢ For generative applications, convolutions still have a lot to offer!
  - And they can keep up with transformers when trained properly… arXiv:2310.16764

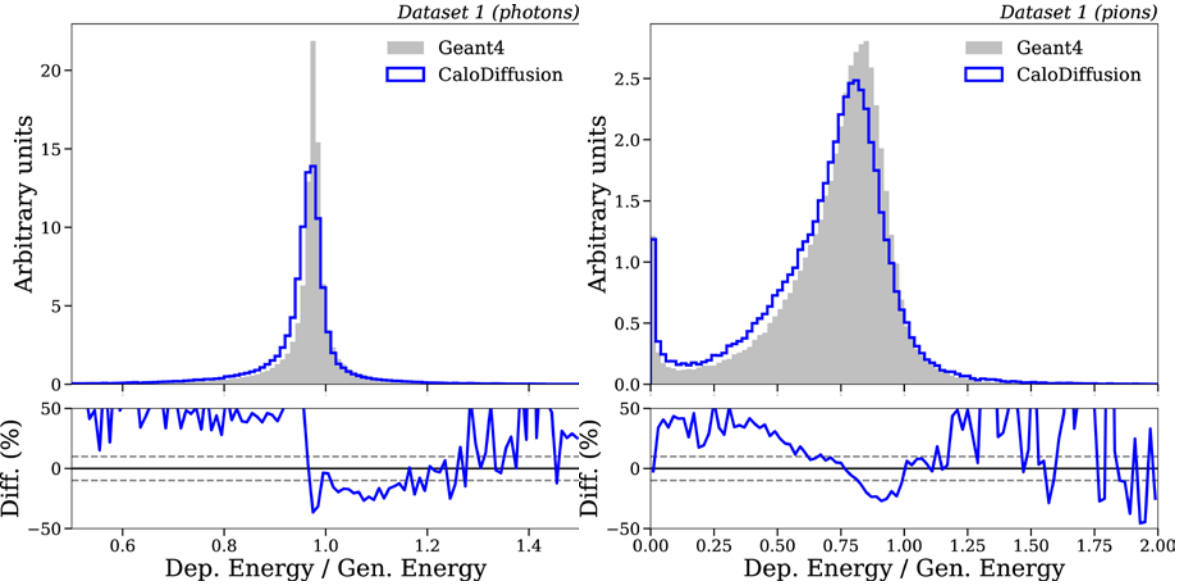
Average Showers

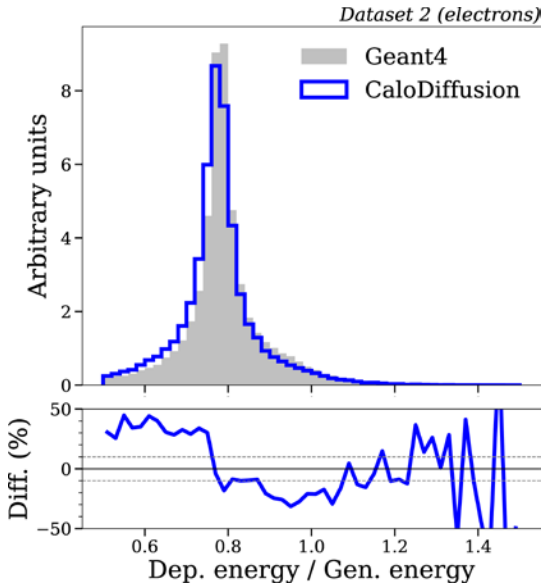


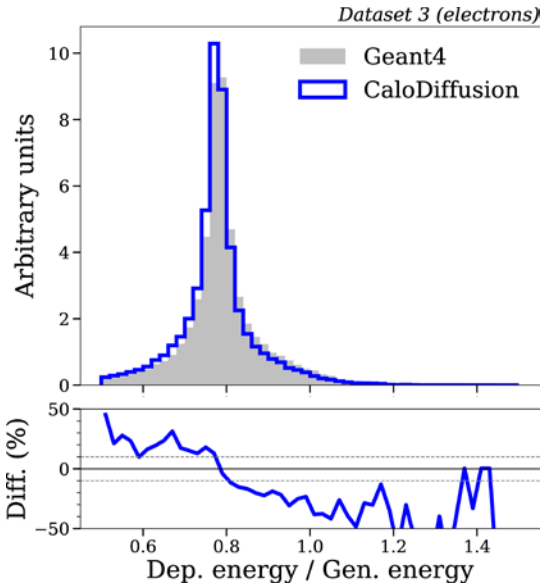
[animated version]

- Top: Geant4; bottom: CaloDiffusion (dataset 1, photons)
  - … or is it the other way around? Can you tell?

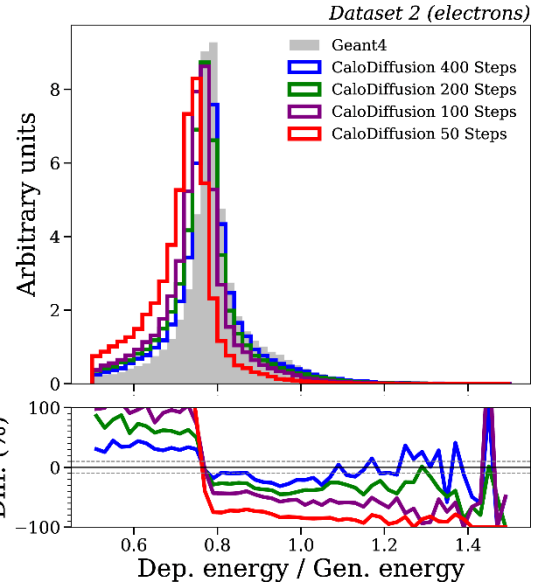
Original CaloDiffusion: Areas for Improvement







- Deficit in total energy modeling
- Need 400 diffusion steps to get acceptable quality
  - Still faster than Geant4 (~100s) w/ batching on GPU
- Fewer steps:
  - Linear speed improvement
  - But even less accurate in this quantity →



Dataset	Batch Size	Time/Shower [s] CPU	GPU
1 (photons) (368 voxels)	1	9.4	6.3
	10	2.0	0.6
	100	1.0	0.1
1 (pions) (533 voxels)	1	9.8	6.4
	10	2.0	0.6
	100	1.0	0.1
2 (electrons) (6.5K voxels)	1	14.8	6.2
	10	4.6	0.6
	100	4.0	0.2
3 (electrons) (40.5K voxels)	1	52.7	7.1
	10	44.1	2.6
	100	-	2.0

Num. Steps	Classifier AUC (low / high)	FPD	E Ratio Sep. Power
400	0.56 / 0.55	0.043(1)	0.011
200	0.61 / 0.56	0.046(1)	0.036
100	0.69 / 0.59	0.065(3)	0.079
50	0.83 / 0.67	0.110(4)	0.251