What can AI offer for Simulation at the EIC?

Michelle P. Kuchera | 7 September 2021

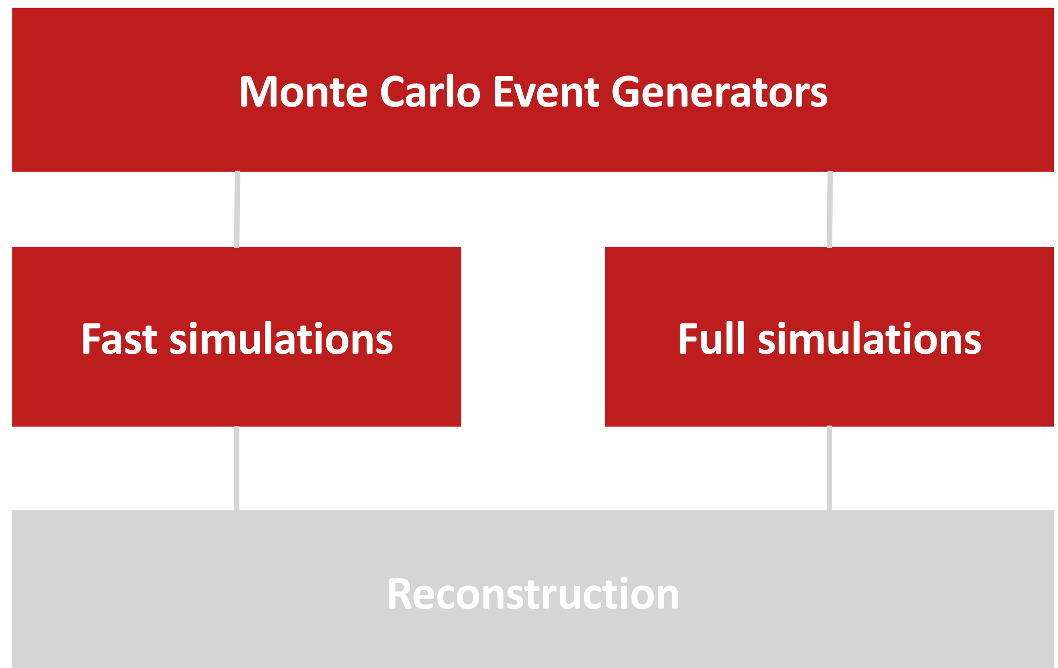
DAVIDSON

Discussion of Event Generation and Simulation Needs

Simulation of physics processes

Simulation of detector responses

Analysis of simulated data

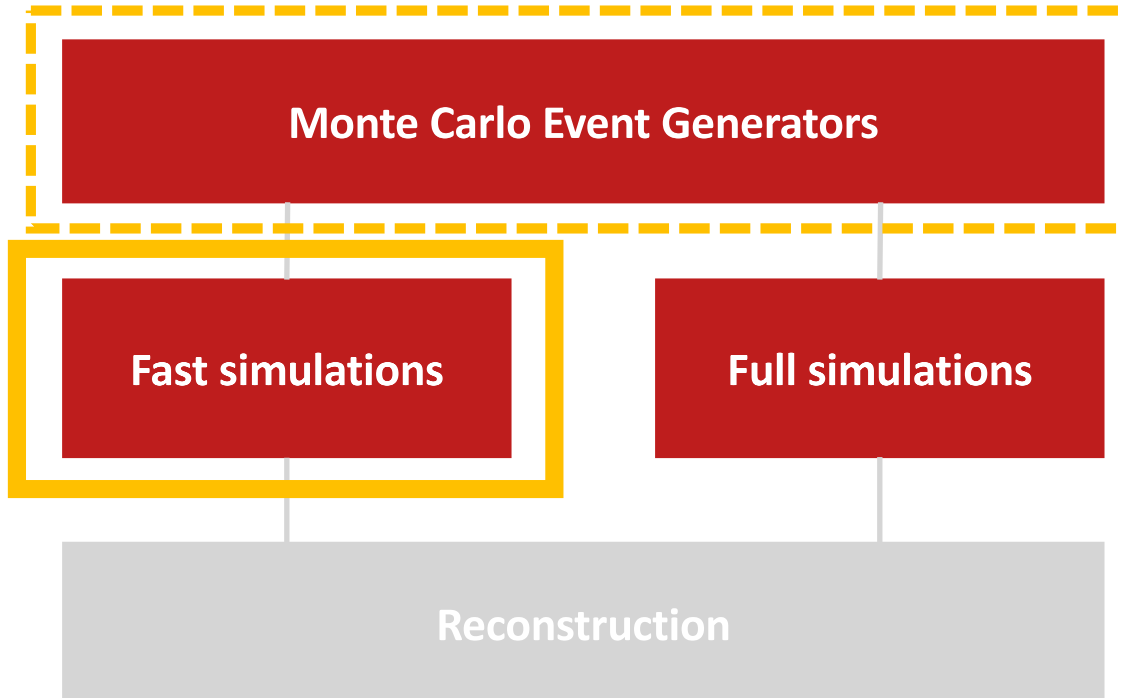


Why AI?

Simulation of physics processes

Simulation of detector responses

Analysis of simulated data

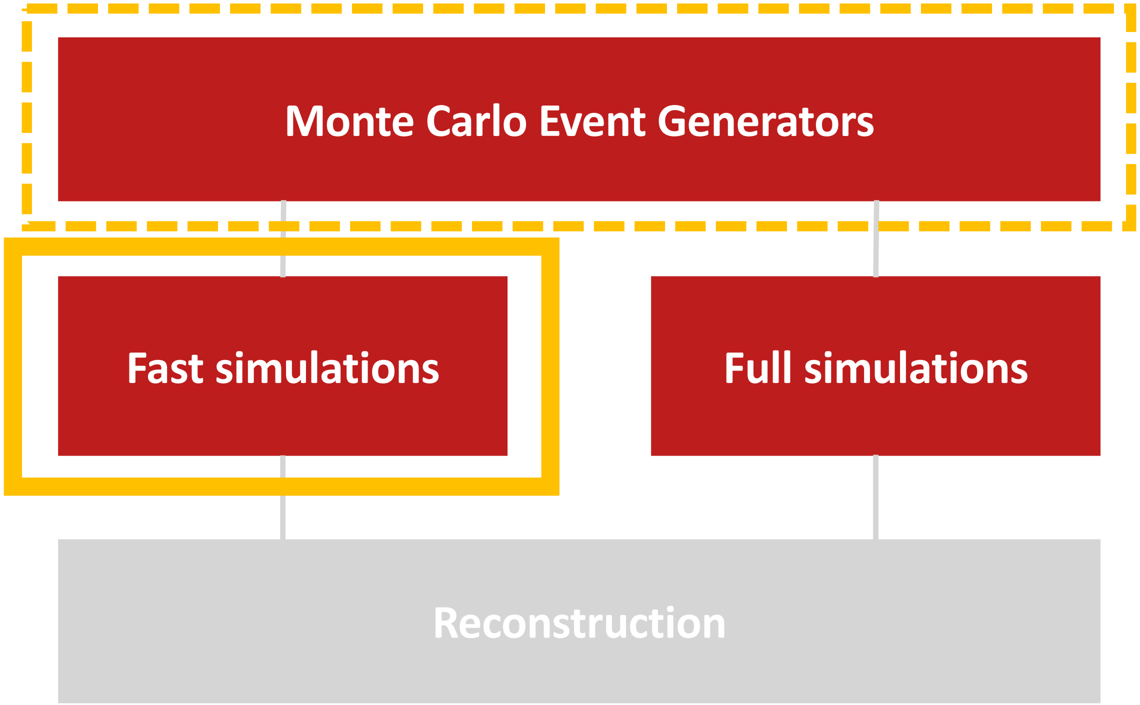


Why AI?

HEPML-LivingReview: A Living Review of Machine Learning for Particle Physics

https://iml-wg.github.io/HEPML-LivingReview/

Generative Networks for LHC events
[2008.08558]



Why AI?

Monte Carlo Event Generators

A Survey of Machine Learning-Based Physics Event Generation
https://www.ijcai.org/proceedings/2021/0588.pdf

MLEGs	Data Source	Detector Effect	Reaction/Experiment	ML Model
[Hashemi *et al.*, 2019]	Pythia8	DELPHES + pile-up effects	$Z \to \mu^+\mu^-$	regular GAN
[Otten *et al.*, 2019]	MadGraph5 aMC@NLO	DELPHES3	$e^+e^- \to Z \to l^+l^-$, $pp \to t\bar{t}$	VAE
[Butter *et al.*, 2019]	MadGraph5 aMC@NLO		$pp \to t\bar{t} \to (bq\bar{q}')(\bar{b}\bar{q}q')$	MMD-GAN
[Di Sipio *et al.*, 2019]	MadGraph5, Pythia8	DELPHES + FASTJET	$2 \to 2$ parton scattering	GAN+CNN
[Ahdida *et al.*, 2019]	Pythia8 + GEANT4		Search for Hidden Particles (SHiP) experiment	regular GAN
[Alanazi *et al.*, 2020b] [Velasco *et al.*, 2020]	Pythia8		electron-proton scattering	MMD-WGAN-GP, cGAN
[Martnez *et al.*, 2020]	Pythia8	DELPHES particle-flow	proton collision	GAN, cGAN
[Gao *et al.*, 2020]	Sherpa		$pp \to W/Z + n$ jets	NF
[Howard *et al.*, 2021]	MadGraph5 + Pythia8	DELPHES	$Z \to e^+e^-$	SWAE
[Choi and Lim, 2021]	MadGraph5 + Pythia8	DELPHES	$pp \to b\bar{b}\gamma\gamma$	WGAN-GP

Table 1: List of existing MLEGs.

Why AI?

Simulation-based inference methods for particle physics
[2010.06439]

Analysis of simulated data

Reconstruction

ML-based event generators

A Survey of Machine Learning-Based Physics Event Generation
https://www.ijcai.org/proceedings/2021/0588.pdf

MLEGs	Data Source	Detector Effect	Reaction/Experiment	ML Model
[Hashemi *et al.*, 2019]	Pythia8	DELPHES + pile-up effects	$Z \to \mu^+\mu^-$	regular GAN
[Otten *et al.*, 2019]	MadGraph5 aMC@NLO	DELPHES3	$e^+e^- \to Z \to l^+l^-$, $pp \to t\bar{t}$	VAE
[Butter *et al.*, 2019]	MadGraph5 aMC@NLO		$pp \to t\bar{t} \to (bq\bar{q}')(\bar{b}\bar{q}q')$	MMD-GAN
[Di Sipio *et al.*, 2019]	MadGraph		$\to$ 2 parton scattering	GAN+CNN
[Ahdida *et al.*, 2019]	Pythia8 + (		arch for Hidden Parti- s (SHiP) experiment	regular GAN
[Alanazi *et al.*, 2020b] [Velasco *et al.*, 2020]	Pythia8		ectron-proton scattering	MMD-WGAN-GP, cGAN
[Martnez *et al.*, 2020]	Pythia8	DELPHES particle-flow	proton collision	GAN, cGAN
[Gao *et al.*, 2020]	Sherpa		$pp \to W/Z + n$ jets	NF
[Howard *et al.*, 2021]	MadGraph5 + Pythia8	DELPHES	$Z \to e^+e^-$	SWAE
[Choi and Lim, 2021]	MadGraph5 + Pythia8	DELPHES	$pp \to b\bar{b}\gamma\gamma$	WGAN-GP

Autoencoders

Table 1: List of existing MLEGs.

ML-based event generators

A Survey of Machine Learning-Based Physics Event Generation
https://www.ijcai.org/proceedings/2021/0588.pdf

MLEGs	Data Source	Detector Effect	Reaction/Experiment	ML Model
[Hashemi *et al.*, 2019]	Pythia8	DELPHES + pile-up effects	$Z \to \mu^+\mu^-$	regular GAN
[Otten *et al.*, 2019]	MadGraph5 aMC@NLO	DELPHES3	$e^+e^- \to Z \to l^+l^-$, $\to t\bar{t}$	VAE
[Butter *et al.*, 2019]	MadGraph		$\to t\bar{t} \to (bq\bar{q}')(\bar{b}\bar{q}q')$	MMD-GAN
[Di Sipio *et al.*, 2019]	MadGraph		$\to$ 2 parton scattering	GAN+CNN
[Ahdida *et al.*, 2019]	Pythia8 +		arch for Hidden Parti-es (SHiP) experiment	regular GAN
[Alanazi *et al.*, 2020b] [Velasco *et al.*, 2020]	Pythia8		ectron-proton scattering	MMD-WGAN-GP, cGAN
[Martnez *et al.*, 2020]	Pythia8	DELPHES particle-flow	proton collision	GAN, cGAN
[Gao *et al.*, 2020]	Sherpa		$pp \to W/Z + n$ jets	NF
[Howard *et al.*, 2021]	MadGraph5 + Pythia8	DELPHES	$Z \to e^+e^-$	SWAE
[Choi and Lim, 2021]	MadGraph5 + Pythia8	DELPHES	$pp \to b\bar{b}\gamma\gamma$	WGAN-GP

Generative Adversarial Networks

Table 1: List of existing MLEGs.

A Survey of Machine Learning-Based Physics Event Generation
https://www.ijcai.org/proceedings/2021/0588.pdf

ML-based event generators

MLEGs	Data Source	Detector Effect	Reaction/Experiment	ML Model
[Hashemi *et al.*, 2019]	Pythia8	DELPHES + pile-up effects	$Z \to \mu^+\mu^-$	regular GAN
[Otten *et al.*, 2019]	MadGraph5 aMC@NLO	DELPHES3	$e^+e^- \to Z \to l^+l^-$, $pp \to t\bar{t}$	VAE
[Butter *et al.*, 2019]	MadGraph5 aMC@NLO		$pp \to t\bar{t} \to (bq\bar{q}')(\bar{b}\bar{q}q')$	MMD-GAN
[Di Sipio *et al.*, 2019]	MadGraph [illegible]	[illegible]	[illegible] $\to$ 2 parton scattering	GAN+CNN
[Ahdida *et al.*, 2019]	Pythia8 + [illegible]	[illegible]	[illegible]arch for Hidden Parti-[illegible]s (SHiP) experiment	regular GAN
[Alanazi *et al.*, 2020b] [Velasco *et al.*, 2020]	Pythia8	[illegible]	[illegible]ectron-proton scattering	MMD-WGAN-GP, cGAN
[Martnez *et al.*, 2020]	Pythia8	DELPHES particle-flow	proton collision	GAN, cGAN
[Gao *et al.*, 2020]	Sherpa		$pp \to W/Z + n$ jets	$\boxed{\text{NF}}$
[Howard *et al.*, 2021]	MadGraph5 + Pythia8	DELPHES	$Z \to e^+e^-$	SWAE
[Choi and Lim, 2021]	MadGraph5 + Pythia8	DELPHES	$pp \to b\bar{b}\gamma\gamma$	WGAN-GP

Normalizing Flows

Table 1: List of existing MLEGs.

Variational Autoencoders

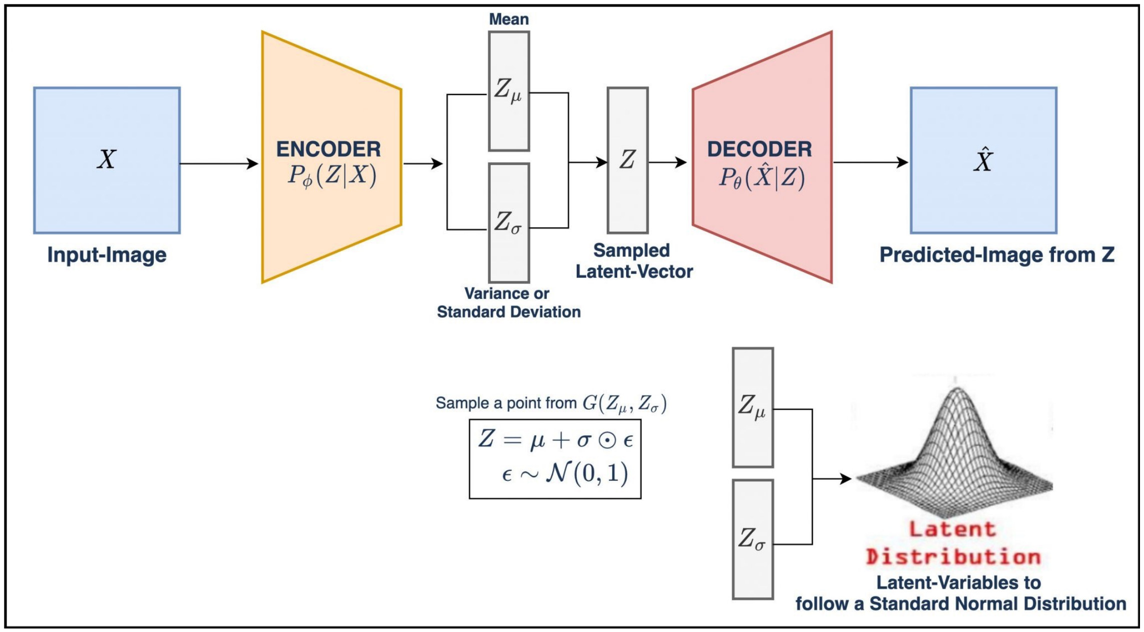
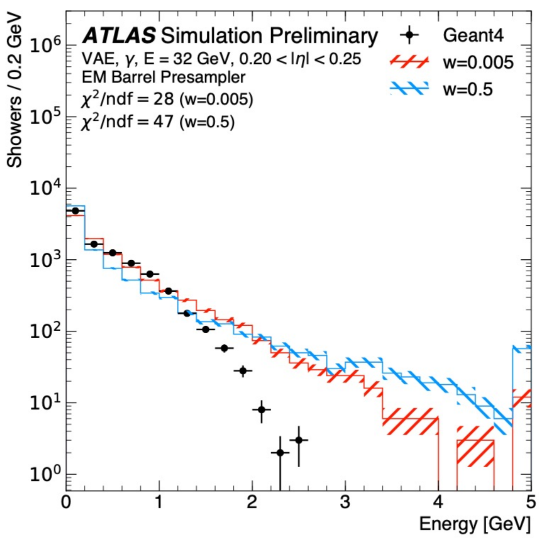


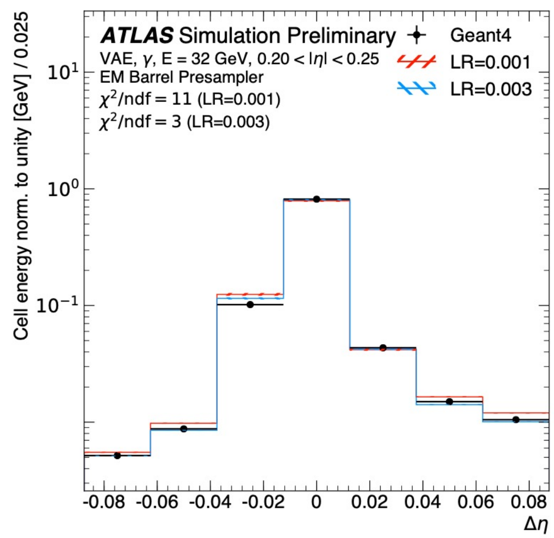
Image credit: Aditya Sharma

Examples in HEP/NP

- photon showers in high-granularity calorimeter. [2005.05334][2102.12491]
- Jet simulation: [2009.04842]
- Fast shower simulation in EM barrel calorimeter: [ATL-SOFT-PUB-2018-001]
- Zero Degree Calorimeters of ALICE [2006.06704]
- On graph structures: reconstruction of calorimeter data [2104.01725]

Variational Autoencoders





Examples in HEP/NP

- photon showers in high-granularity calorimeter. [2005.05334][2102.12491]
- Jet simulation: [2009.04842]
- **Fast shower simulation in EM barrel calorimeter: [ATL-SOFT-PUB-2018-001]**
- Zero Degree Calorimeters of ALICE [2006.06704]
- On graph structures: reconstruction of calorimeter data [2104.01725]

Variational Autoencoders

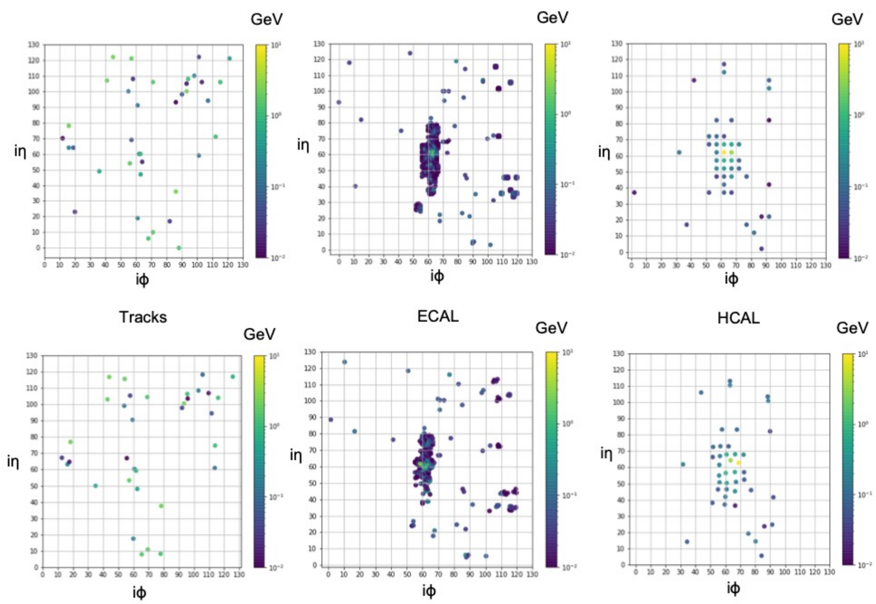


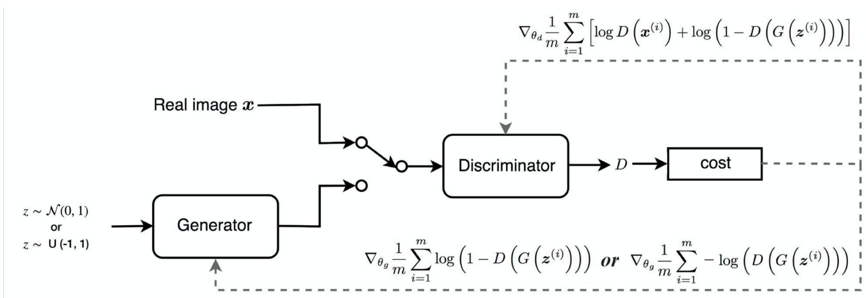
FIG. 3. Original simulated top quark initiated jet (top) compared to the GVAE-reconstructed jet (bottom) in each of the three channels. The energy range is log-scaled for better visualization.

Examples in HEP/NP

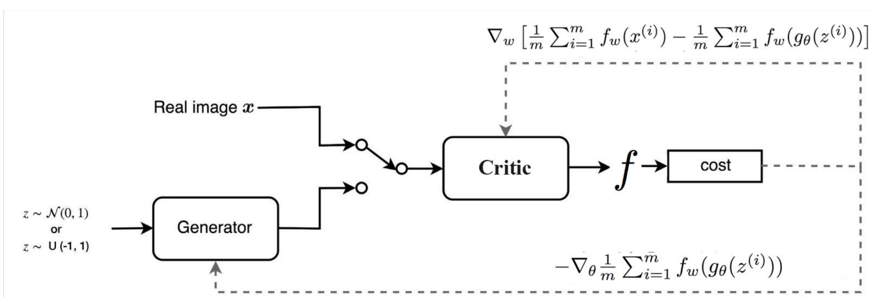
- photon showers in high-granularity calorimeter. [2005.05334][2102.12491]
- Jet simulation: [2009.04842]
- Fast shower simulation in EM barrel calorimeter: [ATL-SOFT-PUB-2018-001]
- Zero Degree Calorimeters of ALICE [2006.06704]
- **On graph structures: reconstruction of calorimeter data [2104.01725]**

Generative Adversarial Networks

GAN (DCGAN)



WGAN

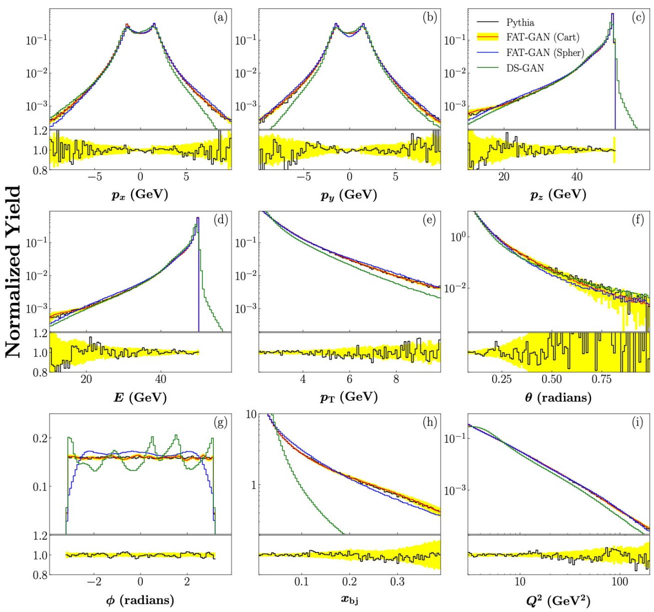


Generative models / density estimation

- GANs:
  - Learning Particle Physics by Example: Location-Aware Generative Adversarial Networks for Physics Synthesis [DOI]
  - Accelerating Science with Generative Adversarial Networks: An Application to 3D Particle Showers in Multilayer Calorimeters [DOI]
  - CaloGAN : Simulating 3D high energy particle showers in multilayer electromagnetic calorimeters with generative adversarial networks [DOI]
  - Image-based model parameter optimization using Model-Assisted Generative Adversarial Networks [DOI]
  - How to GAN Event Subtraction [DOI]
  - Particle Generative Adversarial Networks for full-event simulation at the LHC and their application to pileup description [DOI]
  - How to GAN away Detector Effects [DOI]
  - 3D convolutional GAN for fast simulation
  - Fast simulation of muons produced at the SHiP experiment using Generative Adversarial Networks [DOI]
  - Lund jet images from generative and cycle-consistent adversarial networks [DOI]
  - How to GAN LHC Events [DOI]
  - Machine Learning Templates for QCD Factorization in the Search for Physics Beyond the Standard Model [DOI]
  - DijetGAN: A Generative-Adversarial Network Approach for the Simulation of QCD Dijet Events at the LHC [DOI]
  - LHC analysis-specific datasets with Generative Adversarial Networks
  - Generative Models for Fast Calorimeter Simulation.LHCb case [DOI]
  - Deep generative models for fast shower simulation in ATLAS
  - Regressive and generative neural networks for scalar field theory [DOI]
  - Three dimensional Generative Adversarial Networks for fast simulation
  - Generative models for fast simulation
  - Unfolding with Generative Adversarial Networks
  - Fast and Accurate Simulation of Particle Detectors Using Generative Adversarial Networks [DOI]
  - Generating and refining particle detector simulations using the Wasserstein distance in adversarial networks [DOI]
  - Generative models for fast cluster simulations in the TPC for the ALICE experiment
  - RICH 2018 [DOI]
  - GANs for generating EFT models [DOI]
  - Precise simulation of electromagnetic calorimeter showers using a Wasserstein Generative Adversarial Network [DOI]
  - Reducing Autocorrelation Times in Lattice Simulations with Generative Adversarial Networks [DOI]
  - Tips and Tricks for Training GANs with Physics Constraints
  - Controlling Physical Attributes in GAN-Accelerated Simulation of Electromagnetic Calorimeters [DOI]
  - Next Generation Generative Neural Networks for HEP
  - Calorimetry with Deep Learning: Particle Classification, Energy Regression, and Simulation for High-Energy Physics
  - Calorimetry with Deep Learning: Particle Simulation and Reconstruction for Collider Physics [DOI]
  - Getting High: High Fidelity Simulation of High Granularity Calorimeters with High Speed
  - AI-based Monte Carlo event generator for electron-proton scattering
  - DCTRGAN: Improving the Precision of Generative Models with Reweighting [DOI]
  - GANplifying Event Samples
  - Graph Generative Adversarial Networks for Sparse Data Generation in High Energy Physics
  - Simulating the Time Projection Chamber responses at the MPD detector using Generative Adversarial Networks
  - Explainable machine learning of the underlying physics of high-energy particle collisions
  - A Data-driven Event Generator for Hadron Colliders using Wasserstein Generative Adversarial Network [DOI]
  - Reduced Precision Strategies for Deep Learning: A High Energy Physics Generative Adversarial Network Use Case [DOI]
  - Validation of Deep Convolutional Generative Adversarial Networks for High Energy Physics Calorimeter Simulations
  - Compressing PDF sets using generative adversarial networks

Generative Adversarial Networks

Event generation



e^-+ p scattering

FAT-GAN: Y. Alanazi, et. al. IJCAI-21

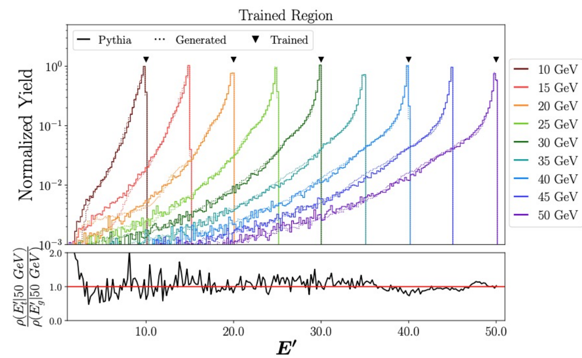
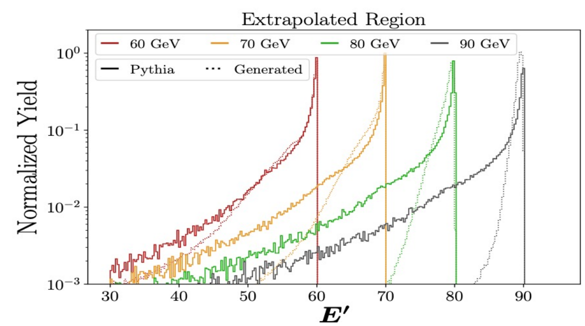


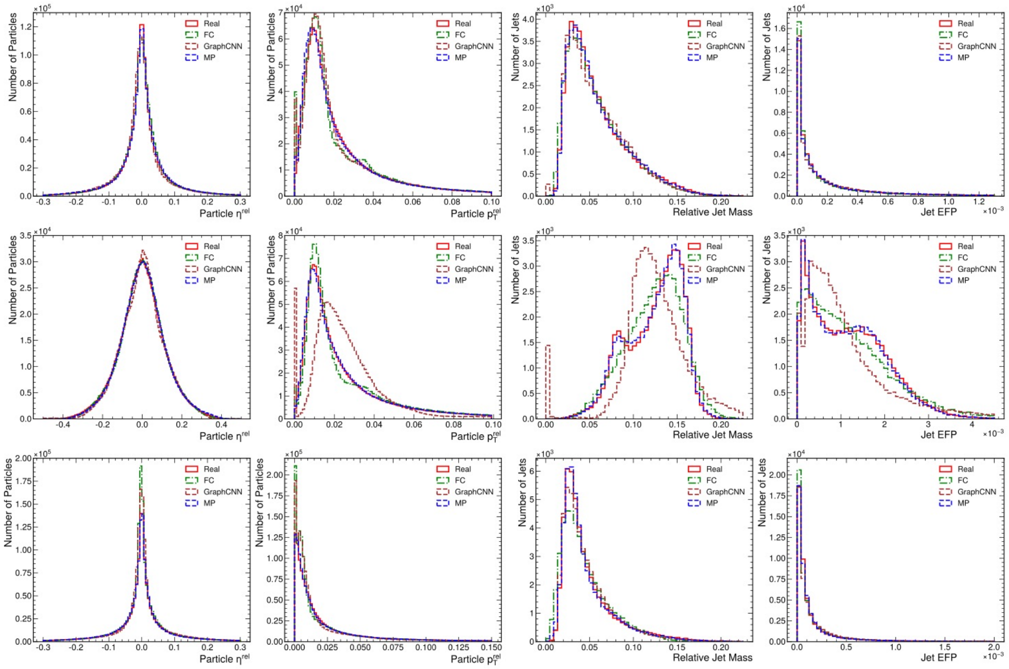
Fig. 2. Comparison of the synthetic (dotted) and true (solid) E' distributions at reaction energies: $E = 10, 15, 20, 25, 30, 35, 40, 45, 50\ GeV$. The black triangles specify the trained energy levels.



cFAT-GAN: L. Velasco, et. al. ICMLA-21

Generative Adversarial Networks

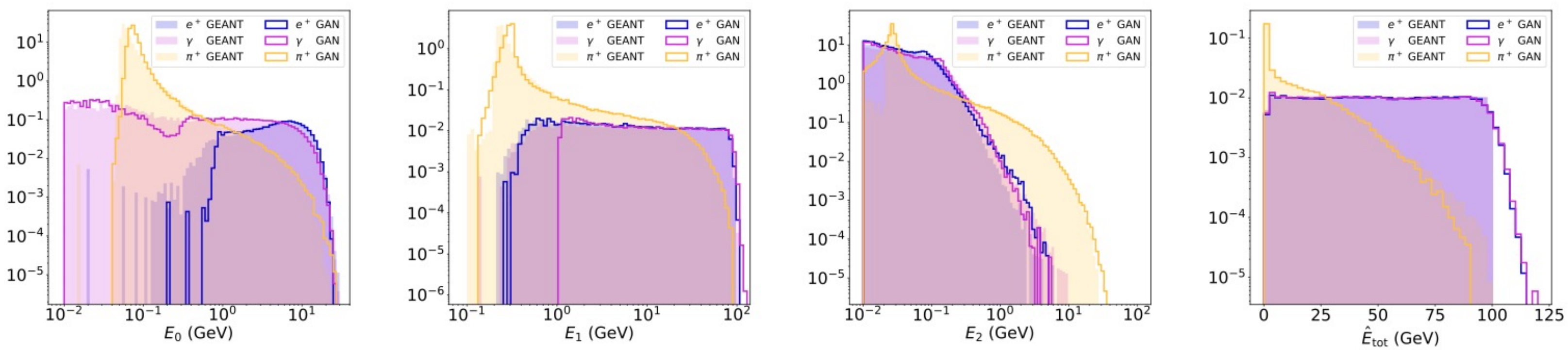
Event generation



Point-cloud GAN
Kansal, et. Al [2106.11535]

Generative Adversarial Networks

Simulation



caloGAN (ATLAS)
Paganini, et. al [1712.10321]

Silicon- Tungsten calorimeter of the proposed International Large Detector
Buhmann , et. al [2005.05334]

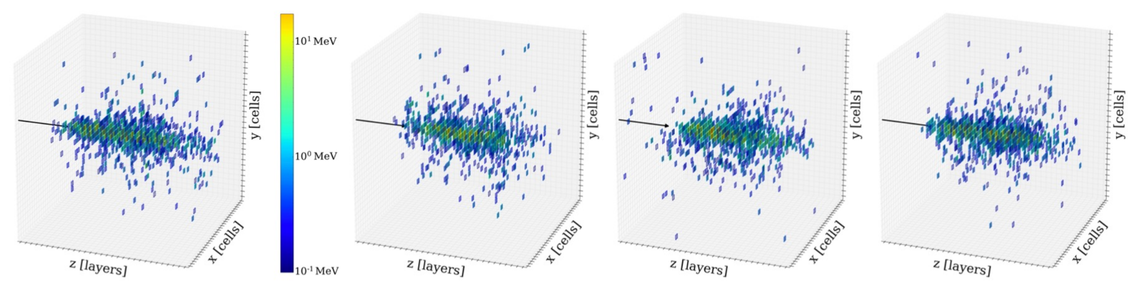
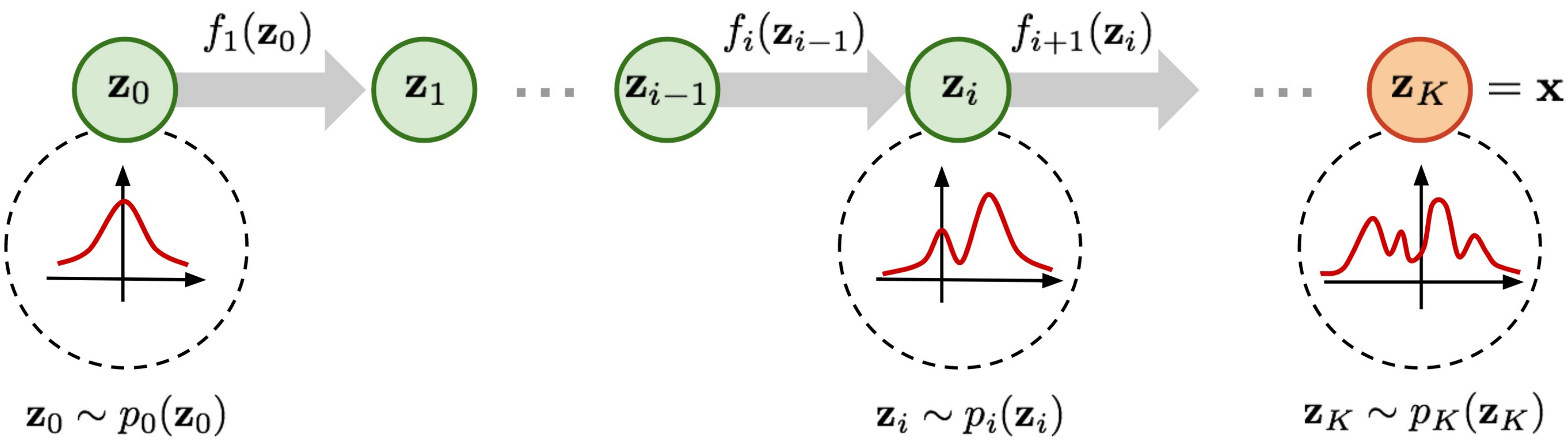


Fig. 5 Examples of individual 50 GeV photon showers generated by Geant4 (left), the GAN (center left), WGAN (center right), and BIB-AE (right) architectures. Colors encode the deposited energy per cell.

Normalizing Flows



Maps complex distributions by transforming a probability density through a series of invertible mappings.

Normalizing Flows

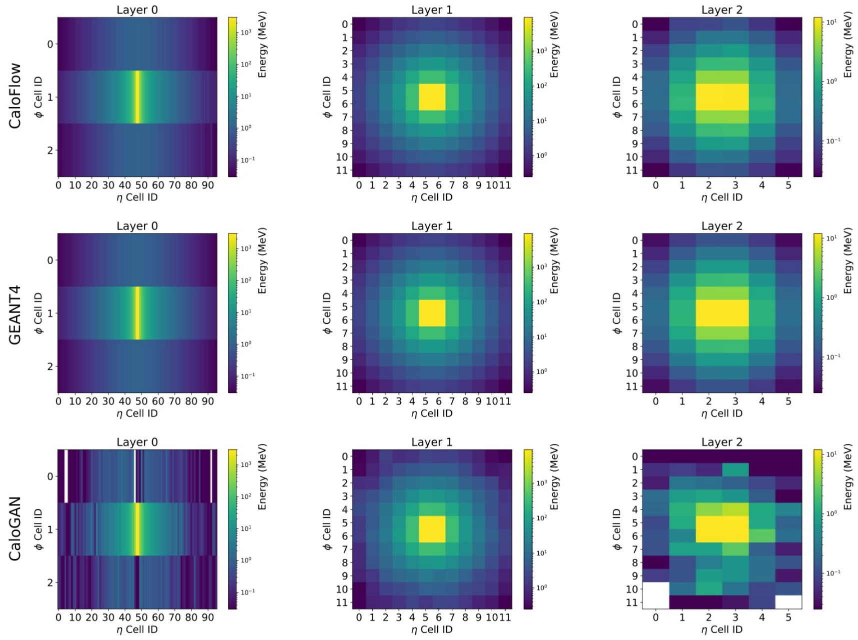


Figure 5. Average shower shapes for e^+. Columns are calorimeter layers 0 to 2, top row shows CaloFlow, center row Geant4, and bottom row CaloGAN

caloFLOW (simplified ATLAS)
Krause, et. al [2106.05285]

Future Directions for EIC simulations?

- **Rare opportunity** to align AI goals early (like in this workshop)
- **Cohesive effort** towards community use. Benchmark points.
- **Look towards powerful generative models** a la natural language models: giant trained models that can be fine tuned
- **Engage with** the computer science / data science communities as collaborators.
- **Rethink workflow.** Can we train models to map p(detector|event gen params)?

Common Software Effort

EIC User Group

Steering Committee

Software Working Group

Proto-Collaborations

ATHENA

CORE*

ECCE

Simulation Working Groups

liaisons

* CORE adapts existing software for their needs and has a far smaller software effort than other proto-collaborations.

HEP Community

Collaboration with **Geant4** and **HEP Software Foundation**

Data Science Community

- EIC as a driver for research in CS and applied math
- scientific, systematic approach to AI / ML approaches to NP
- activation functions, DNN design particular for NP
- building efficient DNNs no more complex than necessary

Common Software Effort

EIC User Group

Steering Committee

Software Working Group

Proto-Collaborations

ATHENA | **CORE*** | **ECCE**

Simulation Working Groups

liaisons

* CORE adapts existing software for their needs and has a far smaller software effort than other proto-collaborations.

HEP Community

Collaboration with **Geant4** and **HEP Software Foundation**

Data Science Community

- EIC as a driver for research in CS and applied math
- scientific, systematic approach to AI / ML approaches to NP
- activation functions, DNN design particular for NP
- building efficient DNNs no more complex than necessary

Engaging the data science community in AI simulation efforts

Interesting testing ground for generative models

- Model meaningful, non-standard distributions
- Physics-embedded metrics for evaluating models

Uniquely structured data

- Event generators: continuous variables of variable length
- Detector simulation: highly structured with correlations
- Interfaces between representations
- Uncertainty quantification: stochastic processes, statistical, systematic uncertainties

Data Science Community

- EIC as a driver for research in CS and applied math
- scientific, systematic approach to AI / ML approaches to NP
- activation functions, DNN design particular for NP
- building efficient DNNs no more complex than necessary

Engaging the data science community in AI simulation efforts

Interesting testing ground for generative models

- Model meaningful, non-standard distributions
- Physics-embedded metrics for evaluating models

Uniquely structured data

- Event generators: continuous variables of variable length
- Detector simulation: highly structured with correlations
- Interfaces between representations
- Uncertainty quantification: stochastic processes, statistical, systematic uncertainties

Data Science Community

Engage as collaborators

Engaging the data science community in AI simulation efforts

Field moving away from hypertuning image and language models

- We have unique data and challenges

Uniquely structured data

- Event generators: continuous variables of variable length
- Detector simulation: highly structured with correlations
- Interfaces between representations
- Uncertainty quantification: stochastic processes, statistical, systematic uncertainties

Data Science Community

Engage as collaborators

Michelle Kuchera
mikuchera@davidson.edu

Summary

- **Ai has the potential for large impacts on Simulation for the EIC.**
- **Large body** of prior related work. Often at “bleeding edge” of AI research. Less commonly used for simulation in practice. Requires work.
- **Simulation R&D** is most efficiently done in common projects and in collaboration with other fields, e.g., HEP or data science.
- **Do not expect replacement** of core tools, e.g., general-purpose MCEGs or Geant4.