

#TLDR

- CERN uses Large Hadron Collider (LHC) to study fundamental matter properties in High Energy Physics experiments.
- Understanding and analysing these experiments requires running complex simulations which are computationally very demanding.
- Leveraging generative machine learning provides an efficient alternative to existing approaches.
- We focus on simulating the Zero Degree Calorimeter (ZDC) in the ALICE experiment, exploring multiple approaches
- Joint Generative Adversarial Networks model speeds up the simulation process by generating data for multiple calorimeter devices simultaneously.
- Conditional diffusion models offer dynamic simulation quality control.
- Conditional control mechanism allows for independent control over generated output.

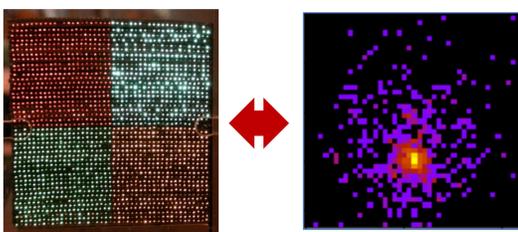
Simulation overview



ALICE TPC

Simulation input:
Particle parameters

Simulation output : ZDC response



Photons deposited in a fiber grid

1- channel pixel image

Zero Degree Calorimeter



Figure 1. Fast simulation overview

Take-aways

- Machine learning generative models provide an efficient alternative to current simulation methods used in High Energy Physics experiments at CERN.
- Joint model reduces inference time by ~50% while providing sample generation quality comparable to separate models
- For diffusion models the number of denoising steps used during inference introduces a natural mechanism to control simulation time and quality trade-off.
- Advanced control mechanisms allow for precise control of the generated outcome, increasing the fidelity of the simulation.

Joint model for simulating multiple calorimeter devices simultaneously

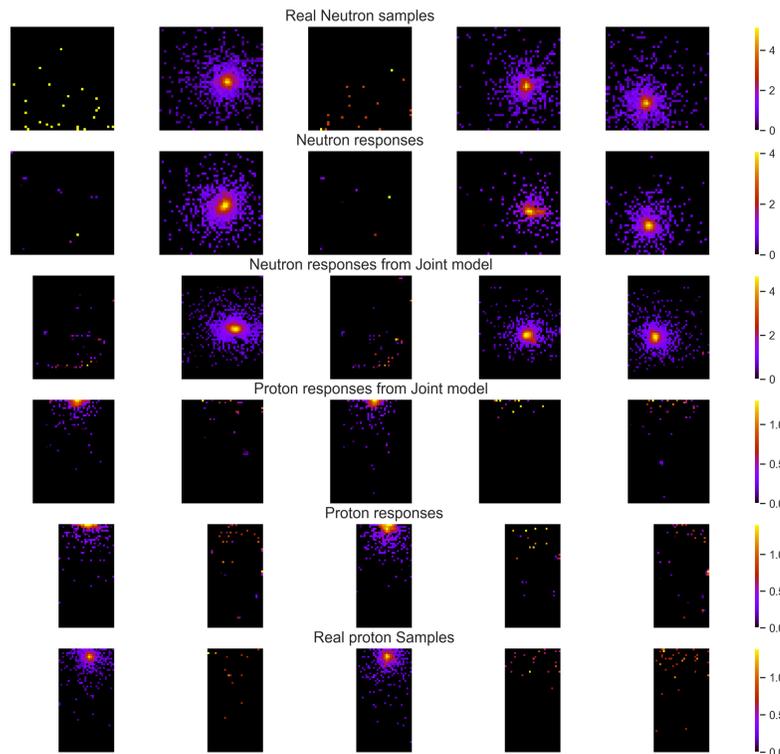


Figure 2. ZDC response simulation examples

- The solution employs a modified SDI-GAN architecture which differs from the standard conditional GAN by accounting for different levels of variance of samples corresponding to different conditional inputs.
- The proposed system has two separate outputs for the generator and two separate inputs and outputs for the discriminator.
- Joint model achieves competitive results relative to distinct models.
- Joint model provides efficient inference significantly speeding up generation of samples.
- The utilization of a single model for multiple calorimeter devices optimizes the simulation process, simplifies integration and reduces overall complexity.
- This approach leverages inherent correlations of data samples from two calorimeter devices making the extraction of shared features more straightforward.

Model	WS dist.	Exec. time [s]
Proton Model	8.91	8.91
Neutron Model	9.01	10.63
Proton part - Joint	6.69	
Neutron part - Joint	8.76	9.39

Table 1. Wasserstein distance metric between original data distribution and models' predictions with execution time

Controlling simulation quality using conditional diffusion model

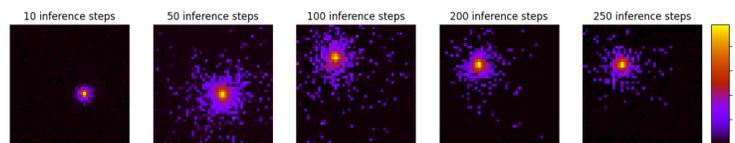


Figure 3. ZDC response simulation examples

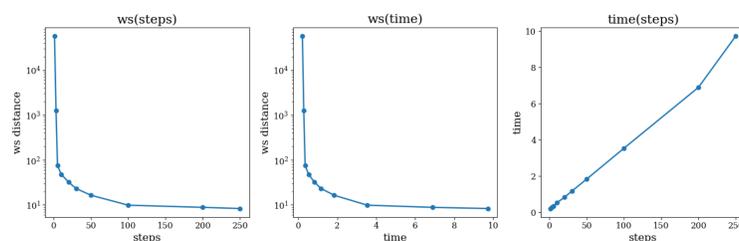


Figure 4. Relations between the number of denoising steps, simulation time and simulation quality

- The solution employs a conditional diffusion model based on a modified 2D U-Net convolutional network architecture.
- Conditional diffusion model offer control on simulation's quality based on a value of inference steps parameter.
- Figure 4 illustrates a trend wherein the incremental adjustment of inference steps parameter is associated with a progressive reduction in Wasserstein Distance.
- Diffusion models present desirable properties such as high distribution coverage and a distinct variety in generated simulations.

Manipulating ZDC response parameters through the modified CorrVAE model

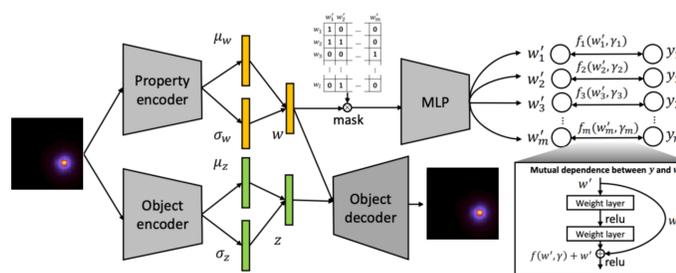


Figure 5. CorrVAE schema

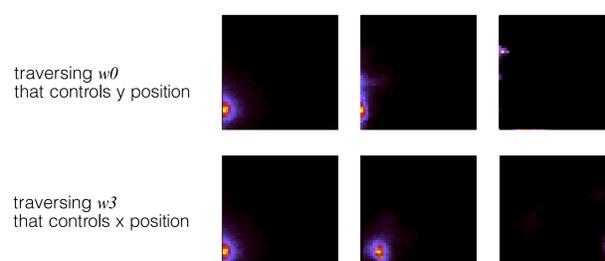


Figure 6. Examples of controlling simulation output properties

- CorrVAE encodes the information of correlated properties into the latent space w and other information of the object into z via the property and the object encoder, respectively.
- The correlation among properties is captured by the mask pooling layer, where the information to predict a specific property is aggregated into the bridging latent variable w_0 .
- We reconstructed this approach using our ZDC response data.
- Results are shown in Figure 6 - we can see that traversing w_0 moves our response up and down and traversing w_3 from left to right.