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Physics-Guided Evaluation and Regularization of Diffusion Models for Calorimeter Simulation

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Fast calorimeter simulation requires accurate generative models and meaningful measures of physical fidelity. We integrate physics-supervised distributional evaluation and residual regularization into our conditional diffusion pipeline for the first time. Shower generation is conditioned on particle entry coordinates and momentum, allowing the model to represent variations in detector response across incident-particle configurations.

The evaluation uses a Frechet Physics Distance - FPD - computed in a representation learned by a network trained to predict particle kinematics and shower-shape observables. Comparing the means and covariance matrices of reference and generated embeddings connects mathematical distributional assessment with physically relevant features, complementing PRD-based scores and KL-divergence diagnostics. Physics supervision guides feature learning towards quantities relevant to shower characterization, while the covariance comparison incorporates correlations between learned features. The diffusion model predicts clean shower maps in a logarithmic energy representation, with a timestep-weighted penalty on negative predictions added to its reconstruction objective. This introduces a soft nonnegativity constraint during training while retaining DDIM sampling without a physics solver.

On the validation sample, the revised pipeline achieves an FPD of 0.058 after clipping negative deposits, compared with 0.889 under the same evaluation protocol. Both Energy and Physical PRD AUC scores exceed 0.999, with the latter evaluated on events with finite shower-shape features. PRD is computed on raw outputs, preserving a separate assessment before clipping. Explicit audits additionally examine negative deposits, sparsity, and total deposited energy, identifying discrepancies not fully reflected in aggregate scores. These checks help distinguish agreement in the selected feature spaces from physical admissibility of individual generated showers. The resulting framework supports systematic model comparison and targeted improvements to calorimeter simulation, with controlled ablations needed to isolate the contribution of residual regularization.

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