

Generative Diffusion Models for Physics Simulation of High-Energy to Multi-Physics Systems: A Brief Survey

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Abstract— Generative diffusion models (GDMs) have emerged as powerful alternatives to traditional physics simulators, offering stable training, high fidelity, and scalability across scientific domains. While numerous applications have been developed in high-energy physics, fluid dynamics, and climate science, the literature remains fragmented. A survey is needed to systematically compare architectures, conditioning strategies, evaluation protocols, and reported results. This paper presents a brief survey of GDMs in scientific simulation. We analyse three representative models—CaloClouds, Jet Diffusion, and the Multi-Physics Diffusion Model (MPDM)—and extend the discussion to emerging domains such as astrophysics, quantum systems, materials science, and geophysics. Comparative tables summarize reported metrics and constraints, while a taxonomy of challenges highlights data scarcity, physical fidelity, generalization, and integration with existing workflows. Finally, we propose open research directions including hybrid physics–ML architectures, uncertainty-aware diffusion, domain adaptation, and real-time deployment.

Index Terms— generative diffusion models, physics-informed ML, high-energy physics, multi-physics, scientific machine learning.

I. INTRODUCTION

High-fidelity simulations are indispensable in modern science. From calorimeter showers in particle detectors to turbulent fluid flows, they drive discovery and enable predictive modelling. However, tools such as GEANT4 in high-energy physics [1] and OpenFOAM in computational fluid dynamics [2] are computationally expensive, limiting scalability and real-time applicability. Generative diffusion models (GDMs) [3], [4] have recently emerged as a promising alternative. By progressively denoising random noise, GDMs produce realistic samples while offering training stability and mode coverage superior to GANs [5]. Their flexibility allows conditioning on physical variables, enabling fast and physically consistent simulations. Despite rapid progress, research remains siloed across domains. High-energy physicists focus on calorimeter and jet simulations, Fluid dynamicists investigate resolution enhancement techniques to reconstruct fine-scale turbulence from coarse simulations, while climate scientists investigate weather downscaling. There is no single survey unifying these works for the broader community.

Contributions of this paper are:

- Provide the first structured survey of GDMs for scientific simulation.
- Compile reported results into comparative tables.
- Analyze architectures, conditioning strategies, and physics-informed training.

- Propose a taxonomy of challenges and highlight open research opportunities.

II. THEORETICAL BACKGROUND

A. Diffusion Models

Diffusion models learn to reverse a Markovian forward process that gradually corrupts data with Gaussian noise:

$$q(x_t|x_{t-1}) = \mathcal{N}(x_t; \sqrt{1 - \beta_t}x_{t-1}, \beta_t I)$$

The reverse process is parameterized by a neural network, trained to predict noise and denoise iteratively [3].

B. Conditioning Strategies

Conditioning enables GDMs to respect scientific context:

- CaloClouds: particle type and energy.
- Jet Diffusion: momentum, particle counts.
- MPDM: coarse simulation fields.

C. Physics-Informed Training

Outputs must obey conservation laws and PDE constraints. Physics-informed diffusion models introduce an additional loss term:

$$\mathcal{L}_{physi} = ||f(\hat{u})||^2$$

where $f(u) = 0$ represents governing equations (e.g., Navier–Stokes). This ensures generated outputs remain physically consistent [6].

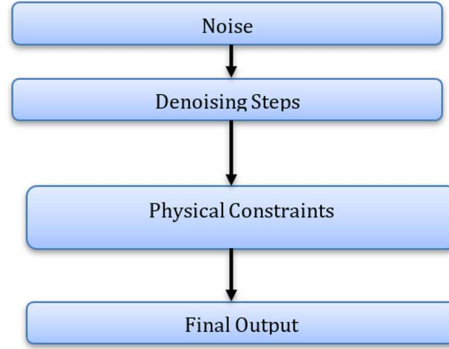


Fig. 1: Diffusion Denoising Schematic

III. GENERATIVE DIFFUSION MODELS IN PHYSICS

A. High-Energy Physics

- CaloClouds [7]: voxel-based 3D U-Net diffusion for calorimeter showers. Achieves 10,000X speedup over GEANT4.
- Jet Diffusion [8]: models jets as unordered sets with permutation-equivariant networks. Achieves 100X speedup, < 2% conservation error.
- Other works: ShowerFlow, Delphes fast simulation integrated with diffusion.

B. Multi-Physics Simulations

- MPDM [9]: super-resolves coarse fields into high-resolution outputs under PDE constraints. Reported +10 dB PSNR, SSIM > 0.9.
- Extensions: climate/weather downscaling [10], spatiotemporal forecasting [11].

C. Cross-Domain Applications

- Astrophysics: cosmic ray showers, telescope map refinement [12].
- Quantum systems: unordered particle states [13].
- Materials science: grain evolution and crack propagation [6].

- Geophysics: seismic mapping, uncertainty quantification.

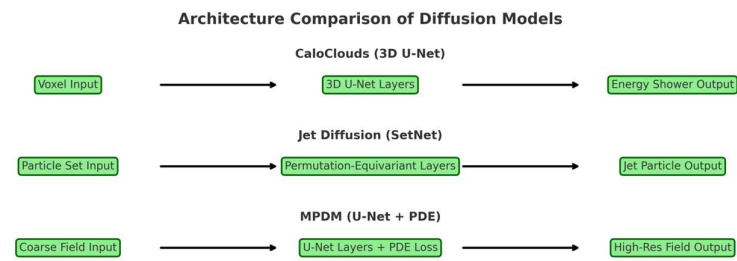


Fig. 2: Architecture comparison diagram

IV. COMPARATIVE ANALYSIS

A. Model Characteristics

TABLE I: MODEL CHARACTERISTICS

Model	Domain	Architecture	Conditioning	Physics Constraint	Benefit
CaloClouds	HEP showers	3D U-Net	Particle energy/type	Post-hoc calibration	10,000× faster than GEANT4
Jet Diffusion	Jets	Permutation-equivariant	Momentum/energy	Conservation terms	100× faster, <2% error
MPDM	Multi-physics	U-Net + PDE residuals	Coarse fields	PDE minimization	+10 dB PSNR, SSIM > 0.9

B. Evaluation Metrics

TABLE II: EVALUATION METRICS REPORTED IN LITERATURE

Model	Metrics Used	Reported Values	Reference
CaloClouds	EMD, energy error	EMD ≈ 0.03 , <5% error	[7]
Jet Diffusion	Chamfer, KL div	KL < 0.05, CD ↓30%	[8]
MPDM	PSNR, SSIM, PDE res.	+10 dB PSNR, SSIM > 0.9	[9]
WeatherBench	RMSE, ACC	RMSE ↓ 15%, ACC ↑ 10%	[10]

C. Domain Suitability

TABLE III: DOMAINS AND BEST-SUITED MODELS

Domain	Best Model	Rationale
Astrophysics	MPDM, CaloClouds	Field refinement and cosmic ray showers
Quantum	Jet Diffusion	Handles unordered particle states
Materials	MPDM	Microscale super-resolution
Geophysics	MPDM	Seismic refinement, uncertainty maps
Climate	MPDM	WeatherBench downscaling, PDE consistency

V. CHALLENGES IN CURRENT LITERATURE

We identify four persistent challenges:

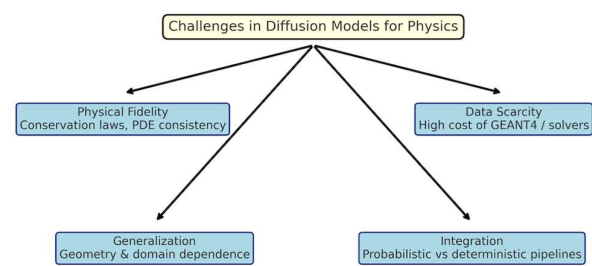


Fig. 3: Taxonomy of Challenges

- Physical fidelity – While diffusion models generate visually and statistically realistic samples, they can sometimes violate fundamental physical laws such as energy conservation, charge conservation, or incompressibility constraints in fluids. For instance, generated calorimeter showers may misrepresent total deposited energy, or fluid velocity fields may not satisfy the Navier–Stokes divergence-free condition. Unlike PINNs [14], which embed constraints explicitly, most current GDMs treat physics only implicitly through training data. Developing physics-constrained diffusion models or post-processing correction mechanisms remains an open problem.
- Data scarcity – Training state-of-the-art GDMs typically requires millions of high-quality samples. However, in science domains, generating labeled data with GEANT4 [1], OpenFOAM [2], or other PDE solvers is computationally prohibitive. For example, simulating particle showers at the LHC can take minutes per event, and running high-resolution climate or CFD simulations requires supercomputing resources. As a result, data scarcity limits the scalability of GDMs in many applications, highlighting the need for data-efficient training (transfer learning, self-supervised pretraining, or physics-guided priors).
- Generalization – Many existing diffusion models are designed for task-specific conditions: CaloClouds [7] for calorimeter showers, Jet Diffusion [8] for particle jets, or MPDM [9] for multiphysics grids. These models often struggle to generalize beyond their training domain, such as to new detector geometries, mesh resolutions, or flow regimes. In contrast, real-world applications (particle physics experiments, aerospace CFD, or astrochemistry) require adaptability to unseen conditions. This limitation motivates research into operator-learning approaches (e.g., FNOs [15]) and meta-learning frameworks [18], [19] that promote cross-domain generalization.
- Integration with Deterministic Simulators - Scientific workflows often rely on deterministic solvers (e.g., GEANT4, CFD codes) for validation and experimental calibration. However, integrating probabilistic outputs of GDMs with such pipelines is non-trivial. For instance, uncertainties from Bayesian diffusion [13] may not directly align with deterministic error bars, and stochastic samples may complicate downstream analysis. Creating hybrid pipelines where GDM surrogates accelerate certain components while solvers enforce ground-truth constraints is a promising but unresolved direction.

VI. OPEN RESEARCH PROBLEMS

Despite rapid progress, several open avenues remain for advancing generative diffusion models (GDMs) in scientific simulation:

- Hybrid Architectures - Future models should integrate complementary architectures such as Physics-Informed Neural Networks (PINNs) [14], Fourier Neural Operators (FNOs) [15], and PDE Transformers [16] with diffusion. PINNs enforce physical constraints directly in the loss, FNOs generalize PDE solution operators across domains, and PDE transformers capture global space–time dependencies. Their integration with diffusion could unify particle-based (e.g., CaloClouds [7], Jet Diffusion [8]) and field-based (e.g., MPDM [9]) simulations, enabling multi-scale hybrid solvers that are both data-driven and physically grounded.
- Uncertainty Quantification - For domains where predictive confidence is as important as accuracy, uncertainty-aware diffusion models are critical. Bayesian diffusion approaches [13] and ensemble-based methods can quantify both epistemic and aleatoric uncertainties. This is particularly vital in astrophysics (e.g., gravitational-wave detection) and climate forecasting (e.g., storm trajectories), where calibrated error estimates directly impact decision-making and risk assessment.
- Domain Adaptation and Few-Shot Transfer- Training diffusion models for every geometry, detector, or flow regime is computationally expensive. Few-shot learning and meta-learning frameworks [18], [19] offer pathways for rapid adaptation, reducing retraining costs. For instance, models trained on LHC jet showers could adapt to next-generation collider environments, or atmospheric models could generalize across planetary systems. Such few-shot transfer would broaden applicability in resource-limited regimes like astrochemistry or hydrology.
- Benchmarking and Reproducibility- While vision and NLP benefit from large, standardized benchmarks, physics ML still lacks broad datasets. Current efforts such as WeatherBench [10] and CaloChallenge [20] provide baselines but cover narrow domains. Expanding benchmarks to include multi-physics interactions (e.g., radiation–hydrodynamics, plasma turbulence) and developing standardized evaluation protocols would strengthen reproducibility and comparability across models. Transparency in hyperparameters, compute budgets, and data splits will be crucial for cross-community adoption.

- **Real-Time Deployment** - A major frontier is deploying diffusion models in real-time digital twins [21]. Applications include adaptive calibration in telescopes, online beam alignment in particle accelerators, or rolling high-resolution climate forecasts. Similarly, engineering twins could use diffusion surrogates for predictive control in aerospace and energy systems. Addressing challenges of latency and hardware efficiency (e.g., model distillation, accelerator-optimized inference) will be necessary to translate diffusion into operational settings.

TABLE IV: RESEARCH GAPS AND SUGGESTED DIRECTIONS

Gap	Suggested Approach	Potential Impact
Lack of constraints	Physics-informed losses	Higher fidelity
Geometry dependence	Meta-learning adaptation	Reusability
Limited datasets	Shared benchmarks	Reproducibility
No uncertainty	Bayesian diffusion	Trustworthiness

VII. CONCLUSION

Generative diffusion models are reshaping scientific simulation by combining statistical learning with physical constraints. This survey consolidates progress across high-energy physics, multi-physics systems, and cross-domain applications. By providing comparative tables, a taxonomy of challenges, and open research directions, we aim to guide both ML researchers entering scientific domains and domain scientists adopting generative approaches.

Future research must address physical fidelity, generalization, and workflow integration. With advances in hybrid architectures, uncertainty-aware modeling, and benchmark datasets, GDMs are poised to become indispensable tools for fast, reliable, and physically consistent simulations.

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