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A Theoretical Framework for Cosmological Field Evolution with Physics-Informed Neural Operators and Geometric Deep Learning

Un Marco Teórico para la Evolución de Campos Cosmológicos con Operadores Neuronales Físicos y Aprendizaje Profundo Geométrico

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ABSTRACT
The large-scale structure (LSS) of the universe poses formidable computational and theoretical challenges for standard cosmological models. We propose a unified theoretical framework that synthesizes six advanced machine learning paradigms to model the evolution of dark matter fields and the dynamics of the cosmic web. This frame-work integrates (1) Neural Operators (NOs) to learn PDE solvers in the continuous limit, (2) Normalizing Flows (NFs) for simulation-based Bayesian inference with exact likelihoods, (3) topological and geometric methods to characterize the structure of the cosmic web, (4) effective field theories (EFTs) and coarse-graining to model multiscale matter dynamics, (5) causal inference to disentangle systematic effects from underlying physics, and (6) geometric autoencoders to learn symmetry-preserving latent representations. We argue that the hybridization of these approaches offers a promising path toward building high-fidelity, computationally efficient, and physically consistent cosmological emulators, capable of overcoming the limitations of current methods and exploiting the wealth of data from upcoming large-scale surveys.

Keywords: cosmology, neural operators, graph neural networks, dark matter

RESUMEN
La estructura a gran escala (LSS) del universo presenta desafíos computacionales y teóricos formidables para los modelos cosmológicos estándar. Proponemos un marco teórico unificado que sintetiza seis paradigmas avanzados de aprendizaje automático para modelar la evolución de campos de materia oscura y la dinámica de la red cósmica. Este marco integra (1) Operadores Neuronales (NO) para aprender resolvedores de Ecuaciones Diferenciales Parciales (EDP) en el límite continuo, (2) Flujos Normalizadores (NF) para inferencia bayesiana basada en simulación con verosimilitudes exactas, (3) métodos topológicos y geométricos para caracterizar la estructura de la red cósmica, (4) teorías de campo efectivas (EFT) y coarse-graining para modelar la dinámica de la materia a múltiples escalas, (5) inferencia causal para desenredar efectos sistemáticos de la física subyacente, y (6) autoencoders geométricos para aprender representaciones latentes que preservan simetrías. Argumentamos que la hibridación de estos enfoques ofrece una ruta prometedora para construir emuladores cosmológicos de alta fidelidad, computacionalmente eficientes y físicamente consistentes, capaces de superar las limitaciones de los métodos actuales y explotar la riqueza de los datos de los próximos sondeos a gran escala.

Palabras clave: cosmología, operadores neuronales, redes neuronales de grafos, materia oscura

INTRODUCTION

The standard model of cosmology, ΛCDM, has been remarkably successful in describing the large-scale structure (LSS) of the universe. However, modelling the nonlinear evolution of cosmic structures, dominated by dark matter and dark energy, remains a significant computational challenge (He *et al.*, 2019; Villaescusa-Navarro *et al.*, 2021). Traditional *N* -body simulations, although accurate, are computationally prohibitive for exhaustive exploration of parameter space and the Bayesian inference required by next-generation surveys such as LSST, Euclid and the Roman Space Telescope.

Machine learning, particularly deep learning, has emerged as a powerful alternative to accelerate simulations and cosmological analysis (Cranmer *et al.*, 2020; Ravanbakhsh *et al.*, 2017; Rojas-Valdivia, 2025). Early efforts focused on convolutional neural networks (CNNs) to analyze two-dimensional mass maps (Jeffrey *et al.*, 2020; Shirasaki *et al.*, 2019) or graph neural networks (GNNs) to analyze the discrete distribution of haloes and galaxies (Villanueva-Domingo & Villaescusa-Navarro, 2022; Garuda *et al.*, 2024). Although promising, these approaches often operate on discretized representations of cosmic fields and may not explicitly enforce physical laws, potentially leading to physically inconsistent predictions.

This article introduces a comprehensive theoretical framework that seeks to close this gap by synthesizing six advanced machine-learning paradigms motivated by physics. Our goal is to lay the foundations for a new generation of cosmological emulators that are not only fast and accurate, but also interpretable and consistent with fundamental physical principles. We propose a hybridization of the following six pillars:

(i) *Neural Operators (NOs):* We frame the evolution of density and cosmological potential fields as an operator learning problem mapping between function spaces. Specifically, we leverage Fourier Neural Operators (FNOs) (Li *et al.*, 2024) and Graph Neural Operators (GNOs) (Kovachki *et al.*, 2023) to learn the solution operator of the Vlasov–Poisson or Schrödinger–Poisson equations. This provides a mesh-free and continuous representation that naturally handles different resolutions and geometries, overcoming the limitations of discrete GNNs (Satorras *et al.*, 2021).

(ii) *Variational inference with normalizing flows (NFs):* We propose to replace approximate likelihoods in simulation-based inference with exact likelihoods learned via continuous normalizing flows (CNFs) and flow-matching techniques (Dax *et al.*, 2023; Lipman *et al.*, 2023). This enables more principled Bayesian inference of cosmological parameters, providing robust uncertainty quantification (Papamakarios *et al.*, 2021; Stachurski *et al.*, 2024).

(iii) *Topological and geometric methods*: The cosmic web possesses a rich topological structure of voids, filaments and clusters. We propose to use persistent homology and Morse theory as a rigorous mathematical language to characterize this structure (Wilding *et al.*, 2021; Sousbie, 2011). Betti numbers and other topological summaries can serve as powerful, physically motivated statistics for cosmological inference (Pranav *et al.*, 2017; Lee & Villaescusa-Navarr0, 2025).

(iv) *Effective field theory (EFT) and coarse-graining:* The dynamics of dark matter are multiscale. We connect GNNs and NOs with the language of the EFT of the LSS (Carrasco *et al.*, 2012; Ivanov, 2022). The neural network learns an effective, coarse-grained representation of the underlying microphysics, analogous to a renormalization-group flow, justifying the model's ability to capture effective dynamics without resolving the fundamental nature of dark-matter particles (Pietroni, 2012).

(v) *Causal representation learning:* A key challenge in cosmology is disentangling physical effects from observational systematics. We advocate the use of causal inference and representation-learning techniques to separate these factors (Schölkopf *et al.*, 2021). This provides a pathway to build models that are robust to selection biases and can identify causal relationships rather than mere correlations (Park *et al.*, 2023).

(vi) *Symmetry-aware geometric autoencoders:* We propose to formalize the notion of a physical latent space using geometric autoencoders that are explicitly designed to preserve fundamental symmetries of the system, such as SE(3) equivariance (Batzner *et al.*, 2022; Winter *et al.*, 2022). This allows the study of cosmological phases and transitions within a low-dimensional manifold endowed with a physically meaningful metric (Chadebec & Allassonnière, 2022; Kneer *et al.*, 2021; Rojas *et al.*, 2024; León *et al.*, 2025).

By integrating these six pillars, we aim to build a holistic theoretical framework that addresses key challenges in modern cosmology: computational cost, physical consistency, interpretability and uncertainty quantification. The following sections elaborate the theoretical underpinnings of each pillar and discuss their potential synergies.

THEORETICAL FRAMEWORK

Neural operators as a unifying continuous framework

The evolution of cosmological fields, such as the matter density contrast $\delta(\mathbf{x}, t)$ and gravitational potential $\phi(\mathbf{x}, t)$, is governed by partial differential equations (PDEs) like the Vlasov–Poisson system. Traditional numerical solvers discretize these fields on a mesh. Graph neural networks (GNNs), though powerful for modelling discrete catalogues of galaxies, inherit this limitation by representing the cosmic web as a discrete graph $G = (V, E)$ (Villanueva-Domingo & Villaescusa-Navarro, 2022). This discretization is not intrinsic to the underlying physics and can introduce artefacts.

We propose elevating this description by recasting the problem in the language of operator learning (Kovachki *et al.*, 2023; Martínez *et al.*, 2024; León *et al.*, 2025). The goal is to learn the solution operator $G^{\dagger}: A \to U$ that maps a set of initial conditions or parameters $a \in A$ to the solution field $u = G^{\dagger}(a) \in U$, where A and U are infinite-dimensional function spaces. This approach is inherently mesh-free and continuous.

From discrete GNNs to continuous operators
A standard message-passing GNN can be viewed as a discrete approximation of an integral operator. The PI-EGNN formalism of the foundational thesis, which uses an equivariant operator $\hat{T}(g \cdot G) = g \cdot \hat{T}(G)$, can be seen as a specific discretization of a continuous operator that preserves symmetries. The convergence of such discrete operators to their continuous counterparts in the limit of infinite nodes ($N \to \infty$) is a crucial theoretical question that can be addressed within the neural-operator framework (Li *et al.*, 2024).

Physics-informed neural operators (PINOs)
We specifically advocate the use of physics-informed neural operators (PINOs) (Li *et al.*, 2024). PINOs combine data-driven learning with physical constraints imposed by the governing PDEs. The loss function for a PINO is a hybrid of a data-based term and a physics-based term:

$$\mathcal{L}(\theta) = \mathcal{L}_{\text{data}}(\theta) + \lambda \mathcal{L}_{\text{phys}}(\theta) \tag{1}$$

where $\mathcal{L}_{\text{data}}$ measures the mismatch between the operator prediction and observed data (e.g., from a low-resolution N-body simulation), and $\mathcal{L}_{\text{phys}}$ penalizes deviations from the PDE residuals, which can be evaluated at much higher resolution (zero-shot super-resolution).

For cosmological applications, the PDE residual could be derived from the Vlasov–Poisson equation. For example, the Fourier Neural Operator (FNO) architecture, a key component of PINO, is particularly well suited for this task. The FNO parametrizes the integral kernel in Fourier space, efficiently capturing global dependencies with a fast Fourier transform (FFT).

$$(\mathcal{K}(a)v)(\mathbf{x}) = \mathcal{F}^{-1}\left(R_{\phi} \cdot (\mathcal{F}v)\right)(\mathbf{x}) \tag{2}$$

where $\mathcal{F}$ denotes the Fourier transform and R_{ϕ} is the learned Fourier representation of the kernel. This formulation has proven highly effective for learning complex dynamics in fluid mechanics and can be applied directly to cosmological fluid evolution (Jamieson *et al.*, 2023; Mishra & Tolley). It provides a formal bridge between discrete GNNs and continuous field evolution, allowing discussions about consistency and convergence. Figure 1 illustrates the architecture of a Fourier Neural Operator.

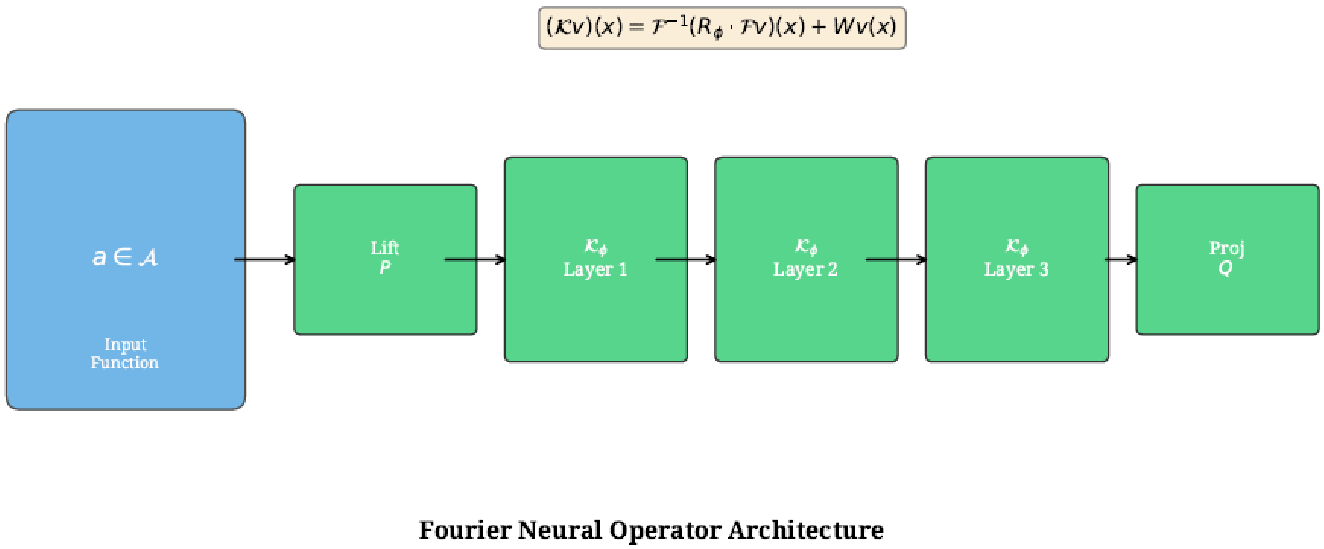

Fig. 1: Architecture of a Fourier Neural Operator (FNO). The input function is lifted to a higher-dimensional representation, processed through iterative Fourier layers that learn global dependencies, and projected back to the output function space.

Exact Bayesian inference with normalizing flows

Inference of cosmological parameters is fundamentally a Bayesian problem: given observed data D, we want to infer the posterior distribution of cosmological parameters θ, $p(\theta|D)$. Bayes' theorem states

$$p(\theta|D) = \frac{p(D|\theta)p(\theta)}{p(D)} \tag{3}$$

where $p(D|\theta)$ is the likelihood, $p(\theta)$ is the prior distribution, and $p(D)$ is the evidence. For complex, nonlinear processes like LSS formation, the likelihood function is intractable. Simulation-based inference (SBI) methods cir-cumvent explicit evaluation of the likelihood by learning a surrogate model from simulations (Cranmer *et al.*, 2020).

However, many SBI techniques rely on approximate likelihoods or posteriors. We propose to harness the power of normalizing flows (NFs) to learn the exact likelihood function, enabling more accurate and reliable inference (Papamakarios *et al.*, 2021).

Learning the likelihood with flows
A normalizing flow is a transformation $f : Z \rightarrow X$ that maps a simple base distribution (e.g., Gaussian) $p_Z(z)$ to a complex target distribution $p_X(x)$ via an invertible and differentiable function. The probability density of a sample $x = f(z)$ can be computed exactly using the change-of-variables formula:

$$p_X(x) = p_Z(f^{-1}(x)) \left|\det\left(\frac{\partial f^{-1}(x)}{\partial x}\right)\right| \tag{4}$$

We can train a conditional NF, $p(D|\theta)$, to learn the likelihood of the data given the parameters by maximizing the log-likelihood of simulated data-parameter pairs. Recent advances such as continuous normalizing flows

(CNFs), based on neural ordinary differential equations (Chen *et al.*, 2018), and flow matching (Lipman *et al.*, 2023; Dax *et al.*, 2023), offer a more flexible and scalable way to train these models, making them suitable for high-dimensional cosmological data (Mootoovaloo *et al.*, 2025; Stachurski *et al.*, 2024).

This approach directly addresses a central challenge in the foundational thesis: computing the evidence ratio $\Lambda(D) = \log[p(D|H_1)/p(D|H_0)]$ for the dark-matter statistical test. Figure 2 illustrates the concept of normalizing flows.

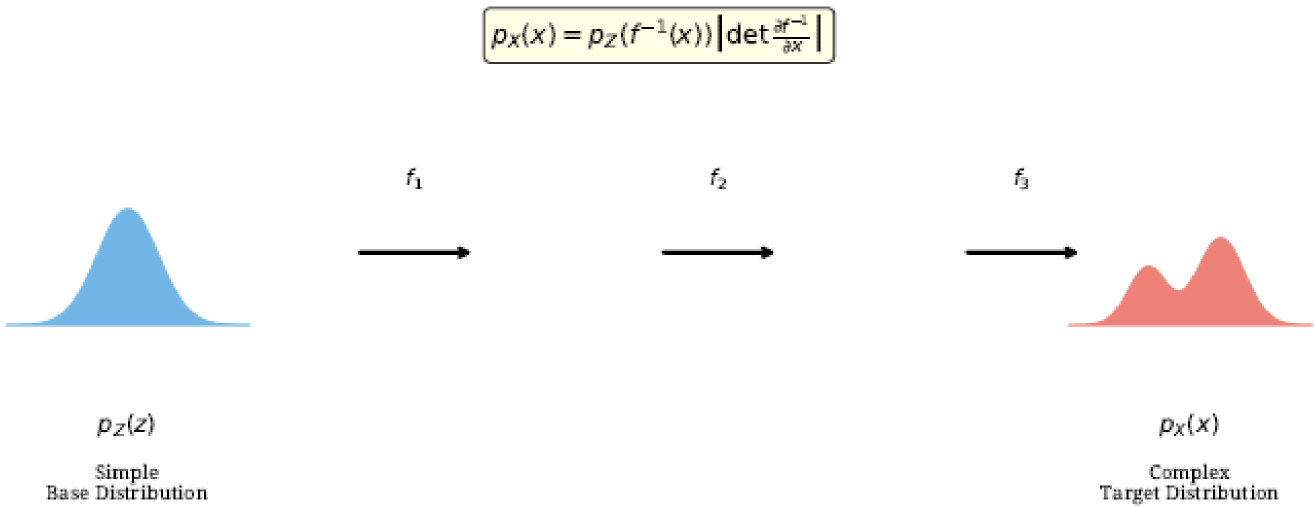

Fig. 2: Normalizing flows transform a simple base distribution (e.g., Gaussian) into a complex target distribution through a sequence of invertible transformations, enabling exact density evaluation.

By learning both likelihoods $p(D|H_1)$ and $p(D|H_0)$ with high fidelity using NFs, we can compute a true Bayes factor, providing a much more solid theoretical foundation for the proposed test and for cosmological model comparison in general.

Topological and geometric characterization of the cosmic web

The cosmic web is a complex network of voids, walls, filaments and clusters. Although visually striking, a rigorous and quantitative description of its morphology and connectivity is challenging. We propose to use tools from topological data analysis (TDA) and geometric measure theory to provide this mathematical foundation (Edelsbrunner & Harer, 2010).

Persistent homology
Persistent homology is a central tool in TDA that captures the topological features of a point cloud or field at multiple scales (Carlsson, 2009). By constructing a sequence of nested topological spaces (a filtration), for example by considering sublevel or superlevel sets of the density field, we can track the birth and death of topological features (connected components, loops, voids). The persistence of these features across scales provides a robust summary of the topology of the data.

The output is typically visualized as a persistence diagram or summarized via Betti numbers $B_k(s)$ as a function of scale s.

- B_0 counts the number of connected components (clusters).
- B_1 counts the number of tunnels or loops (filaments).
- B_2 counts the number of enclosed voids.

These Betti curves have proven to be a powerful cosmological probe, sensitive to parameters such as Ω_m and

σ_8, and to the nature of dark energy and primordial non-Gaussianity (Pranav *et al.*, 2017; Wilding *et al.*, 2021; Pranav *et al.*, 2019).

Connection with Morse theory

Morse theory provides a deep connection between the topology of a manifold and the critical points of a smooth function defined on it. In a cosmological context, the density field can be treated as a Morse function. The critical points of this function correspond to the centers of clusters (maxima), voids (minima) and saddle points that define the filamentary connections (Sousbie, 2011). The persistent cosmic-web formalism (Sousbie *et al.*, 2011) uses this idea to provide a parameter-free definition of cosmic structures. This provides a solid theoretical foundation for constructing the graph in the foundational thesis, where the nodes are haloes and the edges represent physical connections, which can be formally identified as gradient integral lines of the density field connecting the critical points.

Integrating these topological statistics into the feature set of machine-learning models, or using them to define the loss function, can equip the models with a fundamental understanding of large-scale structure that goes beyond local density contrasts (Lee & Villaescusa-Navarro, 2025). Figure 3 illustrates the key concepts of persistent homology applied to the cosmic web.

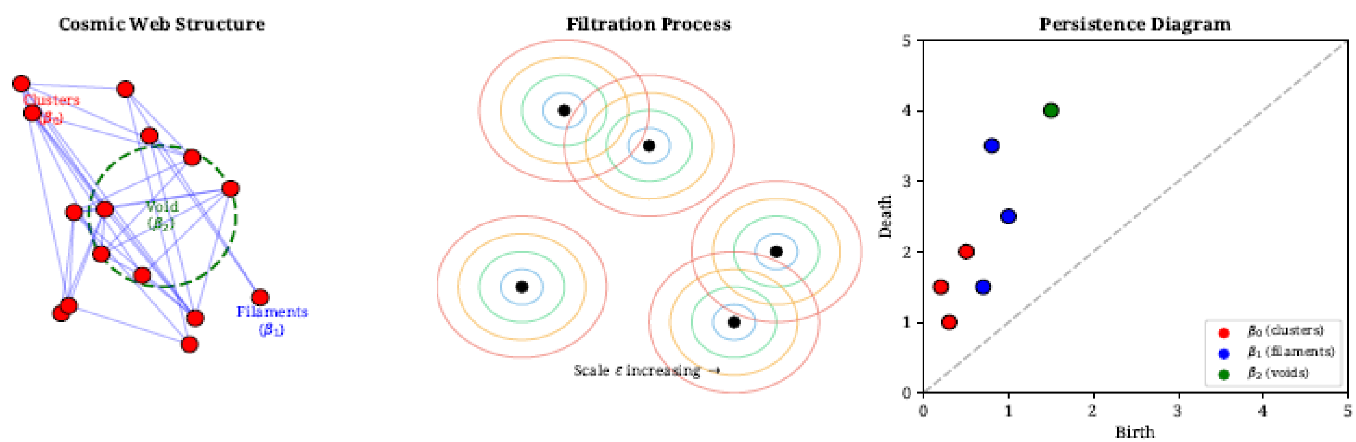

Fig. 3: Topological data analysis of the cosmic web. Left: schematic of the cosmic-web structure showing clusters (β_0), filaments (β_1) and voids (β_2). Centre: Filtration process with growing balls at different scales. Right: Persistence diagram encoding the birth and death of topological features.

Learning effective theories and coarse-graining

A fundamental question is what, precisely, a neural network learns about the dynamics of dark matter. The underlying microphysical nature of dark matter is unknown. We argue that machine-learning models do not need to resolve the ultimate microphysics; instead, they learn an *effective theory* of dark matter's influence on large-scale structure.

This perspective is formalized by the effective field theory of the large-scale structure (EFTofLSS) (Carrasco *et al.*, 2012; Ivanov, 2022). In EFTofLSS, the complex short-wavelength physics is encapsulated in a set of effective stress-tensor terms that modify the fluid equations on large scales. The coefficients of these terms are free parameters fitted to data or simulations.

We propose that a neural operator or GNN, when trained on cosmological simulation data, is implicitly performing a similar task. It learns a non-perturbative, effective closure relation for the fluid equations, capturing the integrated effect of small-scale physics on the large-scale dynamics. This can be viewed as a non-perturbative, data-driven extension of the EFTofLSS program. The network acts as a *coarse-graining* operator, mapping high-entropy initial conditions to the final, large-scale, lower-entropy state, analogous to a renormalization-group (RG) flow (Pietroni, 2012; Uhlemann *et al.*, 2015). This viewpoint provides a powerful conceptual justification: the model is not explaining the micro-nature of dark matter but detecting and modelling its *effective* impact on the cosmic web.

Learning causal representations for robust inference

Standard machine-learning models are powerful correlators but often fail to distinguish correlation from causation. In cosmology this is a critical weakness. For example, the observed light from a galaxy is correlated with the underlying dark-matter mass, but it does not cause it. Moreover, observational data are plagued by systematic effects (e.g., photometric redshift errors, selection biases, intrinsic alignments) that may be correlated with the cosmological signal of interest (Gong *et al.*, 2023).

To build robust models we must move from correlational to causal inference. We propose integrating techniques from causal representation learning (Schölkopf *et al.*, 2021). The goal is to learn representations that are *disentangled*, where distinct latent variables correspond to distinct, independent causal mechanisms in the real world. For example, one latent variable could encode the cosmological parameters (e.g., Ω_m), another could encode baryonic feedback physics, and a third could encode an observational systematic such as dust extinction.

By structuring the model architecture to reflect a causal graph (e.g., cosmology → dark-matter distribution → galaxy properties → observed light), we can train models that are invariant to interventions on specific variables. This would allow us, for example, to infer cosmological parameters that are robust to changes in survey strategy or to marginalize over uncertainties in baryonic physics. This approach provides a rigorous pathway to protect analysis against common criticisms of machine learning as a “black box” that simply exploits spurious correlations in the training data (Park *et al.*, 2023; von Kügelgen, 2024).

Symmetry-aware geometric autoencoders and physical latent spaces

Many machine-learning models for cosmology seek to compress high-dimensional data into a low-dimensional latent space. However, this latent space is often uninterpretable. We propose constructing a *physical latent space* by designing models that explicitly preserve the fundamental symmetries of the physical system.

For cosmology, the key symmetry group is the Euclidean group SE(3), representing translations and rotations. By using SE(3)-equivariant neural networks we ensure that the learned representations transform predictably under these symmetries (Batzner *et al.*, 2022; Satorras *et al.*, 2021). We can use a symmetry-equivariant autoencoder architecture to learn a mapping from the high-dimensional input space (e.g., a galaxy catalogue) to a low-dimensional latent space, and back, respecting these symmetries at every layer (Winter *et al.*, 2022; Nasiri & Bepler, 2022).

This approach, an instance of geometric deep learning (Bronstein *et al.*, 2021), endows the latent space with a meaningful geometric structure. Distances and paths within this space correspond to physical transformations. For example, the latent space could be a manifold where different regions correspond to different cosmological “phases” (e.g., early-stage linear growth versus late-stage nonlinear collapse). Transitions between these phases could be studied as trajectories on this learned manifold. This provides a powerful, interpretable framework for exploring the space of possible cosmological theories and structures, formalizing the concept of a “topological latent space” mentioned in the foundational thesis (Chadebec & Allassonnière, 2022; Kneer *et al.*, 2021; Gabbard *et al.*, 2022).

DISCUSSION AND SYNTHESIS

The six pillars presented above are not independent but deeply interconnected, offering powerful synergies when combined. We envision a unified architecture where these concepts work in concert.

Figure 4 provides a comparative summary of the six theoretical pillars.

Comparative Summary of the Six Theoretical Pillars

Method	Key Concept	Cosmological Application	Key Advantage
Neural Operators (FNO, GNO, DeepONet)	Learn PDE solution operators	Field evolution, N-body emulation	Mesh-free, super-resolution
Normalizing Flows (CNF, Flow Matching)	Exact density estimation	Likelihood-free inference	Exact likelihoods, uncertainty
Topological Data Analysis (Morse, PH)	Multi-scale topology	Cosmic web characterization	Parameter-free, robust
Effective Field Theory (EFT)	Coarse-graining dynamics	Multi-scale modeling	Physical justification
Causal Representation Learning	Disentangle causal factors	Systematic control	Robustness, interpretability
Geometric Autoencoders	Symmetry-preserving latent space	Physical representations	Interpretable, equivariant

Fig. 4: Comparative summary of the six theoretical pillars, highlighting their key concepts, cosmological applications and main advantages.

Figure 5 shows the proposed end-to-end workflow from observations to posterior inference.

End-to-End Workflow: From Observations to Posterior Inference

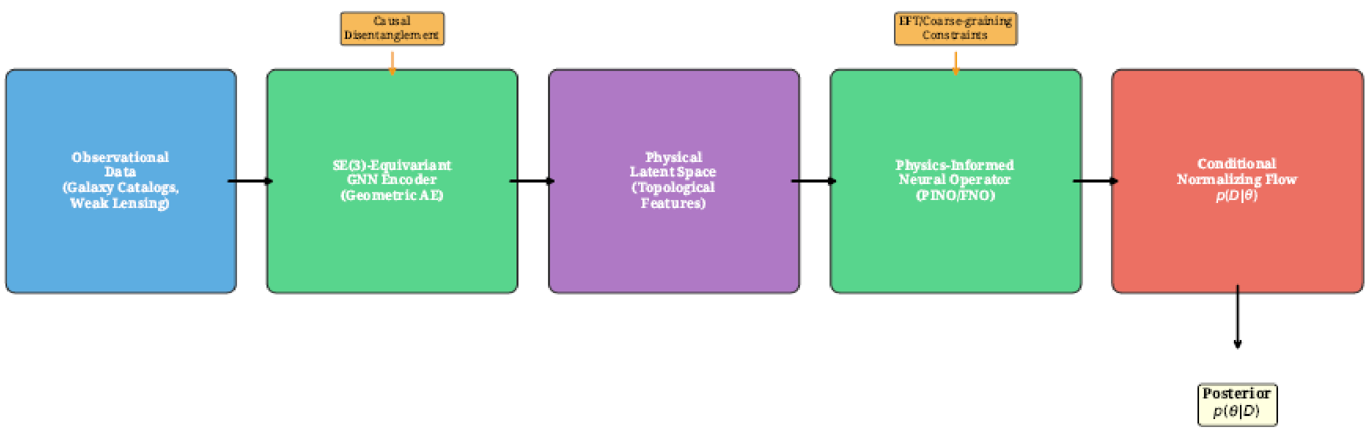

Fig. 5: End-to-end workflow of the proposed framework: observational data are encoded by an SE(3)-equivariant GNN into a physical latent space, evolved by a physics-informed neural operator, and processed by a conditional normalizing flow to obtain the posterior distribution of the cosmological parameters.

- *NOs + TDA:* The continuous fields learned by neural operators can be analysed directly using persistent homology, providing a multiscale topological description of the learned dynamics. Topological features (Betti numbers) can even be used as a loss term to impose a desired topology on the solution.
- *NFs + causal learning:* Normalizing flows can be used to model the distributions of disentangled causal variables, enabling robust, principled inference where the influence of specific physical or systematic effects can be isolated and marginalized.
- *EFT + geometric autoencoders:* The latent space of a symmetry-aware autoencoder can be interpreted as the parameter space of the effective field theory. The autoencoder learns the optimal, non-perturbative coarse-graining of the microphysics into a low-dimensional, physically meaningful representation.
- *GNOs + Morse theory:* The graph structure used by a graph neural operator can be rigorously defined by the Morse-Smale complex of the underlying density field, providing a parameter-free, physically motivated definition of the cosmic-web graph.

Figure 6 illustrates a conceptual diagram of this integrated framework.

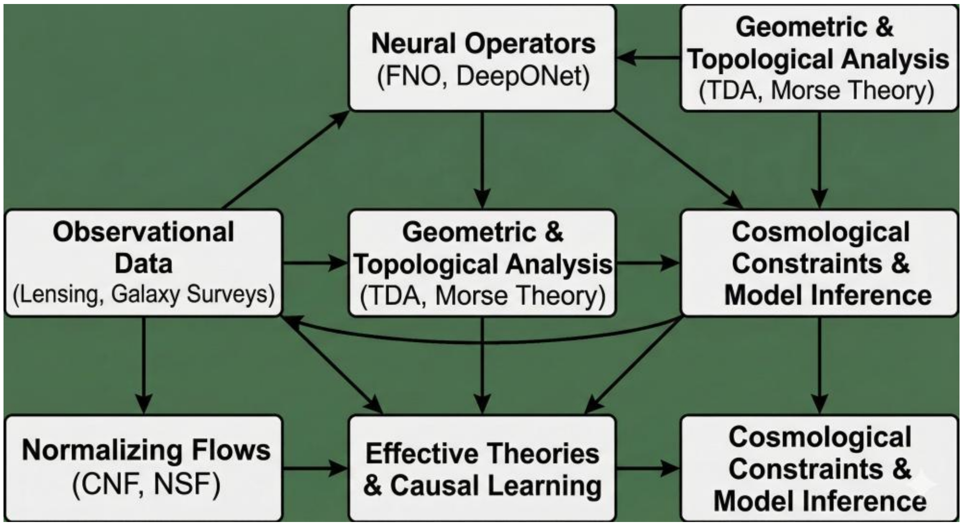

Fig. 6: Unified theoretical framework for AI-driven cosmology, showing the six interconnected pillars: neural operators, normalizing flows, topological data analysis, effective field theory, causal representation learning and geometric autoencoders.

An end-to-end model could involve an SE(3)-equivariant GNN encoding galaxy-catalogue data into a physical latent space. A neural operator then evolves this latent state forward in time, governed by PDE constraints. Finally, a conditional normalizing flow takes this evolved state to compute the exact likelihood for a given set of cosmological and noise parameters, enabling full Bayesian inference.

CONCLUSION

We have presented a unified theoretical framework that synthesizes six leading machine-learning paradigms to address fundamental challenges in computational cosmology. By integrating neural operators, normalizing flows, topological data analysis, effective field theory, causal inference and geometric autoencoders, we have charted a comprehensive roadmap for building the next generation of cosmological emulators.

This framework moves beyond the current correlational, discretization-dependent models toward a new class of emulators that are continuous, physically consistent, causal and uncertainty-aware. The key contributions of this proposed synthesis are:

- A shift from discrete graph representations to continuous, mesh-free operator learning, providing a more fundamental description of field evolution.
- The replacement of approximate likelihoods with exact ones learned via normalizing flows, enabling robust, principled Bayesian inference.
- The formalization of cosmic-web structure using the mathematical language of topology and geometry.
- A justification of deep-learning models as learners of effective theories, connecting them with the established EFT framework and renormalization-group flows.
- A clear pathway to disentangle physical effects from systematics through causal representation learning.
- The construction of interpretable, symmetry-preserving latent spaces that mirror the underlying physics.

Successful implementation of this framework will not only provide new, powerful tools for analyzing data from upcoming surveys, but also deepen our theoretical understanding of the universe, machine learning and the powerful interface between them.

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