Elucidating the Design Choice of Probability Paths in Flow Matching for Forecasting

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Abstract

Flow matching has recently emerged as a powerful paradigm for generative modeling and has been extended to probabilistic time series forecasting. However, the impact of the specific choice of probability path model on forecasting performance, particularly for high-dimensional spatio-temporal dynamics, remains under-explored. In this work, we demonstrate that forecasting spatio-temporal data with flow matching is highly sensitive to the selection of the probability path model. Motivated by this insight, we propose a novel probability path model designed to improve forecasting performance. Our empirical results across various dynamical system benchmarks show that our model achieves faster convergence during training and improved predictive performance compared to existing probability path models. Importantly, our approach is efficient during inference, requiring only a few sampling steps. This makes our proposed model practical for real-world applications and opens new avenues for probabilistic forecasting.

1 Introduction

Generative modeling has achieved remarkable success in recent years, especially for generating high-dimensional objects by learning mappings from simple, easily-sampled reference distributions, π_0, to complex target distributions, π_1. In particular, diffusion models have pushed the capabilities of generating realistic samples across various data modalities, including images (Ho et al., 2020; Song et al., 2020b; Karras et al., 2022), videos (Ho et al., 2022; Blattmann et al., 2023; Gupta et al., 2023), and spatio-temporal scientific data like climate and weather patterns (Pathak et al., 2024; Kohl et al., 2024). Despite their impressive performance, diffusion models often come with high computational costs during training and inference. Additionally, they typically assume a Gaussian reference distribution, which may not be optimal for all data types and can limit modeling flexibility.

One promising alternative is flow matching, where the mappings are learned via a stochastic process that transforms π_0 into π_1 through an ordinary differential equation (ODE), approximating its marginal vector flow (Lipman et al., 2022; Albergo et al., 2023; Liu et al., 2022; Tong et al., 2023b; Pooladian et al., 2023; Lipman et al., 2024). While score-based models (Song & Ermon, 2019; Song et al., 2020a;b; Ho et al., 2020) are specific instances of flow matching, with Gaussian transition densities, the general framework allows for a broader class of interpolating paths. This flexibility can lead to deterministic sampling schemes that are faster and require fewer steps (Zhang & Chen, 2022). Recent work has demonstrated the remarkable capabilities of flow matching models for generating high-dimensional images (Esser et al., 2024) and discrete data (Gat et al., 2024).

Building on this, flow matching in latent space has recently been applied to forecasting spatio-temporal data (Davtyan et al., 2023) (predicting future frames in videos). This approach leverages latent representations to capture the complex dynamics inherent in temporal data. However, spatio-temporal forecasting, especially for videos and dynamical systems data, presents unique challenges. A video prediction model capable of generalizing to new, unseen scenarios must implicitly "understand" the scene: detecting and classifying objects, learning how they move and interact, estimating their 3D shapes and positions, and modeling the physical laws governing the environment (Battaglia et al., 2016). Similarly, accurate weather forecasting

requires capturing intricate physical processes and interactions across multiple scales (Dueben & Bauer, 2018; Schultz et al., 2021).

We observe that, in the context of spatio-temporal forecasting, the performance of flow matching is highly sensitive to the choice of the probability path model, an important topic which has not been widely explored within a unified framework. Different probability paths can significantly impact the accuracy and convergence of forecasting models, particularly when dealing with complex dynamical systems characterized by partial differential equations (PDEs) and chaotic behaviors. Motivated by this, we propose a novel probability path model tailored for probabilistic forecasting of dynamical systems, with a particular focus on PDE datasets relevant to scientific applications. Our model leverages the continuous dynamics intrinsic to spatio-temporal data by interpolating between consecutive sequential samples. This approach ensures better alignment with the constructed flow, leading to improved predictive performance, more stable training, and greater inference efficiency. Existing probability path models often fail to fully capture the continuous nature of spatio-temporal data, resulting in a misalignment with flow-based methods and suboptimal outcomes. Our proposed model addresses these limitations directly.

Building on previous approaches, we provide a theoretical framework and efficient algorithms tailored to probabilistic forecasting of high-dimensional spatio-temporal dynamics using flow matching in latent space. Within this framework, we demonstrate that our probability path model outperforms existing models across several forecasting tasks involving PDEs, achieving faster convergence during training and requiring fewer sampling steps during inference. These advances enhance the practicality of flow matching approaches for real-world applications, particularly in scenarios where computational resources and time are critical constraints. Our main contributions are the following.

- **Theoretical Framework and Efficient Algorithms:** We present a theoretical framework and efficient algorithms for applying flow matching in latent space to the probabilistic forecasting of dynamical systems (see Algorithms 1-2), extending the approach of (Lipman et al., 2022) and (Davtyan et al., 2023). Our approach is specifically tailored for time series data, enabling effective modeling of complex temporal dependencies inherent in dynamical systems.
- **Novel Probability Path Model:** Using dynamical optimal transport and the Schrödinger's bridge perspective (see Theorem 3.2), we motivate and propose a new probability path model (see Section 3.3) specifically designed for modeling dynamical systems data. We provide theoretical insights to show that the variance of the vector field (VF) generating our proposed path can be lower than that of the optimal transport (OT) VF proposed by (Lipman et al., 2022) for sufficiently correlated spatio-temporal samples (see Theorem 3.3). We further provide intuitions to understand why our model leads to smoother training loss curve and faster convergence compared to other models.
- **Empirical Validation:** We provide extensive empirical results to demonstrate that our proposed probability path model can outperform other models on several forecasting tasks involving PDEs (see Section 5). Our results demonstrate that the proposed probability path model outperforms existing flow matching models, achieving faster convergence during training and improved predictive performance across several evaluation metrics, while requiring fewer sampling steps.

2 Flow Matching for Probabilistic Forecasting

In this section, we first introduce the objective of probabilistic forecasting, and then we discuss how flow matching can be used for learning conditional distributions in latent space.

Probabilistic forecasting framework. Suppose that we are given a training set of n trajectories, with each trajectory of length m, $S_n = \{(\mathbf{x}^{1:m})^{(i)}\}_{i=1,\dots,n}$, where $(\mathbf{x}^{1:m})^{(i)} = ((x^1)^{(i)}, \dots, (x^m)^{(i)})$, (with the $(x^l)^{(i)} \in \mathbb{R}^d$), coming from an underlying continuous-time dynamical system. For simplicity, we denote the trajectories as $\mathbf{x}^{1:m} = (x^1, \dots, x^m)$ unless there is a need to specify the corresponding n. The trajectories are observed at arbitrary time points $\mathbf{t}_{1:m} = (t_1, \dots, t_m)$ such that $x^i := x(t_i) \in \mathbb{R}^d$ and $(x(t))_{t\in[t_1,t_m]}$ are the observed states of the ground truth system. In practice, we may have access to only few trajectories, i.e., n is small or even $n = 1$, and the trajectories themselves may be observed at different time stamps.

The goal of probabilistic forecasting is to predict the distribution of the upcoming l elements given the first k elements, where $m = l + k$, i.e.: $q(x^{k+1}, \ldots, x^{k+l}|x^1, \ldots, x^k) = \prod_{i=1}^{l} q(x^{k+i}|x^1, \ldots, x^{k+i-1})$. We propose to model each one-step predictive conditional distribution via a probability density path. Instead of using score-based diffusion models to specify the path, we choose flow matching, a simpler method to train generative models. With flow matching, we directly work with probability paths, and we can simply avoid reasoning about (forward) diffusion processes altogether. Moreover, we shall work in a latent space.

Flow matching in latent space. Let $z^\tau = \mathcal{E}(x^\tau)$ for $\tau = 1, \ldots, m$, where $\mathcal{E}$ denotes a pre-trained encoder that maps from the data space to a lower dimensional latent space. Working in the latent space, our goal is to approximate the ground truth distribution $q(z^\tau|x^1, \ldots, x^{\tau-1})$ by the parametric distribution $p(z^\tau|z^{\tau-1})$, which can then be decoded as $x^\tau = \mathcal{D}(z^\tau)$. The latent dynamics can be modeled by an ODE:

$$\dot{Z}_t = u_t(Z_t), \tag{1}$$

where u_t is the (velocity) VF describing the instantenous rate of change of the state at time t. Learning the dynamics of the system is equivalent to approximating the VF u_t. This can be done by regressing a neural network using the mean squared error (MSE) loss.

Following the idea of flow matching, we infer the dynamics of the system generating $\mathbf{z}$ from the collection of latent observables by learning a time-dependent VF $v_t : [0, 1] \times \mathbb{R}^d \to \mathbb{R}^d$, $t \in [0, 1]$, such that the ODE

$$\dot{\phi}_t(Z) = v_t(\phi_t(Z)), \quad \phi_0(Z) = Z, \tag{2}$$

defines a time-dependent diffeomorphic map (called a flow), $\phi_t(Z) : [0, 1] \times \mathbb{R}^d \to \mathbb{R}^d$, that pushes a reference distribution $p_0(Z)$ towards the distribution $p_1(Z) \approx q(Z)$ along some probability density path $p_t(Z)$ and the corresponding VF $u_t(Z)$. In other words, $p_t = [\phi_t]_* p_0$, where $[\cdot]_*$ denotes the push-forward operation. Here, q is the ground truth distribution, p denotes a probability density path, i.e., $p : [0, 1] \times \mathbb{R}^d \to \mathbb{R}_{>0}$, and $\int p_t(Z)dZ = 1$. We also write $Z_t = \phi(Z)$; and thus the ODE can be written as $\dot{Z}_t = v_t(Z_t), Z_0 = Z$. Typically the reference distribution p_0 is chosen to be the standard Gaussian (Lipman et al., 2022; Liu et al., 2022).

In other words, the main goal of flow matching is to learn a deterministic coupling between p and q by learning a VF v_t such that the solution to the ODE (2) satisfies $Z_0 \sim p$ and $Z_1 \sim q$. When $\mathbf{Z} = (Z_t)_{t\in[0,1]}$ solves Eq. (2) for a given function v_t, we say that $\mathbf{Z}$ is a flow with the VF v_t. If we have such a VF, then (Z_0, Z_1) is a coupling of (p, q). If we can sample from p, then we can generate approximate samples from the coupling by sampling $Z_0 \sim p$ and numerically integrating Eq. (2). This can be viewed as a continuous normalizing flow (Chen et al., 2018).

If one were given a pre-defined probability path $p_t(Z)$ and the corresponding VF $u_t(Z)$ that generates the path, then one could parametrize $v_t(Z)$ with a neural network $v_t^\theta(Z)$, with θ the learnable parameter, and solve the least square regression by minimizing the flow matching loss:

$$\min_\theta \mathcal{L}_{fm}(\theta) := \mathbb{E}_{t,p_t(Z)}\omega(t)\|v_t^\theta(Z) - u_t(Z)\|^2, \tag{3}$$

where $t \in \mathcal{U}[0, 1]$, $Z \sim p_t(Z)$ and $\omega(t) > 0$ is a weighting function. We take $\omega(t) = 1$ unless specified otherwise. However, we do not have prior knowledge for choosing p_t and u_t, and there are many choices that can satisfy $p_1 \approx q$. Moreover, we do not have access to a closed form u_t that generates the desired p_t. We shall follow the approach of (Lipman et al., 2022) and construct a target probability path by mixing simpler conditional probability paths. This probability path is the marginal probability path:

$$p_t(Z) = \int p_t(Z|\tilde{Z})q(\tilde{Z})d\tilde{Z}, \tag{4}$$

obtained by marginalizing the conditional probability density paths $p_t(Z|\tilde{Z})$ over observed latent trajectories $\tilde{Z}$, with $p_0(Z|\tilde{Z}) = p(Z)$ and $p_1(Z|\tilde{Z}) = \mathcal{N}(Z|\tilde{Z}, \epsilon^2 I)$ for a small $\epsilon > 0$. Doing so gives us a marginal probability p_1 which is a mixture distribution that closely approximates q. Then, assuming that $p_t(Z) > 0$ for all Z and t, we can also define a marginal VF as:

$$u_t(Z) = \int u_t(Z|\tilde{Z})\frac{p_t(Z|\tilde{Z})q(\tilde{Z})}{p_t(Z)}d\tilde{Z}, \tag{5}$$

Table 1: Choices of probability density paths that we study in this paper. For VE-diffusion, σ_t is increasing in t, $\sigma_0 = 0$. For VP-diffusion, β = noise scale.

Model	a_t	b_t	c_t^2
VE-diff.	1	0	σ_{1-t}^2
VP-diff.	$e^{-\frac{1}{2}T(1-t)}$	0	$1 - e^{-T(1-t)}, T(t) = \int_0^t \beta(s)ds$
OT-VF	t	0	$(1-(1-\epsilon_{min})t)^2$, $\epsilon_{min} \geq 0$
SI	$1-t$	t or t^2	$\epsilon^2 t(1-t)^2$, $\epsilon > 0$
Ours	$1-t$	t	$\sigma_{min}^2 + \sigma^2 t(1-t)$, $\sigma_{min}, \sigma \geq 0$

where $u_t(Z|\tilde{Z})$ is a conditional VF (conditioned on the latent trajectory $\tilde{Z}$). It turns out that this way of mixing the conditional VFs leads to the correct VF for generating the marginal probability path (4). We can then break down the intractable marginal VF into simpler conditional VFs which depends on a single sample.

To deal with the intractable integrals in Eq. (4)-(5) which complicates computation of an unbiased estimator of $\mathcal{L}_{fm}$, we shall minimize the conditional loss proposed by (Lipman et al., 2022):

$$\min_\theta \mathcal{L}_{cfm}(\theta) := \mathbb{E}_{t,p_t(Z|\tilde{Z}),q(\tilde{Z})}\omega(t)\|v_t^\theta(Z) - u_t(Z|\tilde{Z})\|^2, \tag{6}$$

where $t \in \mathcal{U}[0,1]$, $\tilde{Z} \sim q(\tilde{Z})$, $Z \sim p_t(Z|\tilde{Z})$, and $u_t(Z|\tilde{Z})$ is the VF defined *per sample* $\tilde{Z}$ that generates the conditional probability path $p_t(Z|\tilde{Z})$. Importantly, one can show that the solution of (6) is guaranteed to converge to the same result in (3); see Theorem D.1 in App. D. Therefore, the conditional flow matching loss can match the pre-defined target probability path, constructing the flow that pushes p_0 towards p_1. Since both the probability path and VF are defined per sample, we can sample unbiased estimates of the conditional loss efficiently, particularly so with suitable choices of conditional probability paths and VFs.

3 Probability Path Models for Probabilistic Forecasting

In this section, we describe the family of probability paths that we consider for flow matching, and we propose an improved model tailored for probabilistic forecasting of spatio-temporal data.

3.1 Common Probability Path Models

The family of Gaussian conditional probability paths gives us tractable choices to work with since the relevant quantities in Eq. (6) and thus the conditional flow can be defined explicitly. Therefore, we will work with Gaussian probability paths. Moreover, we are going to solve (6) over the dataset of all transition pairs $\mathcal{D} = \{(z^{\tau-1}, z^\tau)\}_{\tau=2,\ldots,m}$, and use a pair of points for $\tilde{Z}$, setting $\tilde{Z} = (Z_0, Z_1) \in \mathcal{D}$. In particular, we consider the following class of models for the probability paths:

$$p_t(Z|\tilde{Z} := (Z_0, Z_1)) = \mathcal{N}(Z|a_t Z_0 + b_t Z_1, c_t^2 I), \tag{7}$$

where a_t, b_t and c_t are differentiable time-dependent functions on $[0,1]$, and I denotes the identity.

Table 1 provides five different choices of probability paths, including our proposed choice, that we study here. The optimal transport (OT) VF model was initially proposed by (Lipman et al., 2022), and setting $\epsilon_{min} = 0$ gives us the rectified flow model of (Liu et al., 2022), which proposed connecting data and noise on a straight line. The stochastic interpolant (SI) model in Table 1 is the one considered by (Chen et al., 2024). The VE- and VP-diffusion conditional VFs (derived with Theorem D.2) coincide with the VFs governing the Probability Flow ODE for the VE and VP diffusion paths proposed in (Song et al., 2020b). It has been shown that combining diffusion conditional VFs with the flow matching objective leads to a training alternative that is more stable and robust when compared to existing score matching approaches (Lipman et al., 2022).

As remarked in (Lipman et al., 2022), there are many choices of VFs that generate a given probability path. We shall use the simplest VF that generates flow whose map is affine linear. Let $p_t(Z|\tilde{Z})$ be the Gaussian probability path defined in Eq. (7) and consider the flow map ψ_t defined as $\psi_t(Z) := a_t Z_0 + b_t Z_1 + c_t Z$ with

$c_t > 0$. Then the unique VF that defines ψ_t is (see Theorem D.2 and the proof in App. D):

$$u_t(Z|\tilde{Z}) = \frac{c_t'}{c_t}(Z - (a_t Z_0 + b_t Z_1)) + a_t' Z_0 + b_t' Z_1, \tag{8}$$

where prime denotes derivative with respect to t, and $u_t(Z|\tilde{Z})$ generates the Gaussian path $p_t(Z|\tilde{Z})$.

In view of this, minimizing the conditional loss becomes:

$$\min_\theta \mathcal{L}_{cfm}(\theta) := \mathbb{E}_{t,z^\tau,z^{\tau-1},p_t(Z|z^\tau,z^{\tau-1})}\omega(t)\left\| v_t^\theta(Z) - \frac{c_t'}{c_t}(Z - (a_t z^\tau + b_t z^{\tau-1})) - a_t' z^\tau - b_t' z^{\tau-1}\right\|^2, \tag{9}$$

where $t \sim \mathcal{U}[0,1]$, $Z \sim p_t(Z|z^\tau, z^{\tau-1})$ and $\mathbf{z} \sim q(\mathbf{z})$. We refer to this as the Flow Matching loss parametrization and shall work with this parametrization. There are other parametrizations: most popular ones are the Score Matching loss, Score Flow loss and DDPM loss. See App. C for a comparison of different loss parametrizations and App. B for connections to SDE based generative models.

3.2 Optimal Probability Paths

We consider the problem of selecting the optimal probability paths within the class of the Gaussian probability paths. We shall make use of the Schrödinger bridge (Léonard, 2013; Chen et al., 2021b) perspective, and seek to find the *optimal* stochastic processes that evolve a given measure into another, subject to marginal constraints and based on a *prior belief*. This optimal process describes a novel probability path model that we propose for probabilistic forecasting of spatio-temporal data.

To be more precise, let ν, ν' be two given probability measures and let $\mathbb{Q}$ be the path measure of an arbitrary stochastic process. The Schrödinger bridge (SB) is the solution to the following constrained minimization problem over all path measures $\mathbb{P}$ (which are absolutely continuous with respect to $\mathbb{Q}$) of stochastic processes on the finite time interval $[0,1]$:

$$\min_{\mathbb{P}_0=\nu,\ \mathbb{P}_1=\nu'} D_{KL}(\mathbb{P}\|\mathbb{Q}), \tag{10}$$

where D_{KL} denotes the Kullback–Leibler divergence and $\mathbb{P}_t$ denotes the time marginal of $\mathbb{P}$ at time t. Typically ν and ν' are the (empirical) marginal distributions of an unknown continuous-time dynamics observed at the initial and terminal times, and $\mathbb{Q}$ is the path measure of a prior (or reference) process that represents our belief of the dynamics before observing the data. The solution $\mathbb{P}^*$ to the problem can then be interpreted as the optimal dynamics that conforms to the prior belief $\mathbb{Q}$ while respecting the data marginals $\mathbb{P}_0^* = \nu$, $\mathbb{P}_1^* = \nu'$. In other words, the SB is the (path measure of the) finite-time diffusion which admits as initial and terminal distributions the two distributions of interest and is the closest in KL divergence to (the path measure of) a reference diffusion. Recent work (Shi et al., 2024; Pooladian & Niles-Weed, 2024) focuses on developing improved algorithms to solve SB problems for general classes of reference diffusions. SBs have also been used to formulate generative models by interpolating distributions on a finite time interval (Wang et al., 2021; De Bortoli et al., 2021; Chen et al., 2021a; Peluchetti, 2023; Tong et al., 2023a; Liu et al., 2023; Gottwald & Reich, 2024).

We will consider Gaussian prior processes for $\mathbb{Q}$. The Gaussian probability paths that we consider can be formulated via the differential equation: $dZ_t = (\dot{a}_t Z_0 + \dot{b}_t Z_1 + \dot{c}_t \xi)dt$, where $\xi \sim \mathcal{N}(0, I)$. Note that $\mathbb{E}[\dot{Z}_t|Z_0, Z_1] = \dot{a}_t Z_0 + \dot{b}_t Z_1 =: \alpha_t$. We shall take $\mathbb{Q}$ to be the path measure of the linear SDE with drift α_t:

$$dY_t = \alpha_t dt + \omega dW_t,\ t \in [0,1], \tag{11}$$

where $\omega > 0$ is a regularity parameter and W_t is the standard Wiener process. While many choices for $\mathbb{Q}$ exists, the rationale behind our choice is that the Gaussian process Y_t admits a minimal representation $Y_t = \mathbb{E}[Z_t|Z_0, Z_1] + \omega W_t$ that incorporates Brownian motion as a reference noise to characterize the stochasticity surrounding the conditional estimation of Z_t. Importantly, such choice allows interpretation of the SBs as generalized dynamical optimal transport (DOT) (Chewi et al., 2024) between two (not necessarily Gaussian) measures. In particular, adapting Theorem 1 in (Bunne et al., 2023) to our setting, we have:

Proposition 3.1. *Consider the SB problem with Y_t as the reference process:*

$$\min_{\mathbb{P}_0=\nu,\ \mathbb{P}_1=\nu'} D_{KL}(\mathbb{P}\|\mathbb{Y}), \tag{12}$$

where $\mathbb{Y}$ is the path measure induced by $(Y_t)_{t\in[0,1]}$. Then, (12) is equivalent to $\inf_{(\rho_t,v_t)} \mathbb{E}\left[\int_0^1 C(\rho_t, v_t)\, dt\right]$, with

$$C(\rho_t, v_t) := \frac{\|v_t\|^2}{2\omega^2} + \frac{\omega^2}{8}\|\nabla \log \rho_t\|^2 - \frac{1}{2}\langle \alpha_t, \nabla \log \rho_t\rangle, \tag{13}$$

where the infimum is taken over all pairs (ρ_t, v_t) such that $\rho_0 = \nu$, $\rho_1 = \nu'$, ρ_t absolutely continuous, and satisfies $\partial_t \rho_t = -\nabla \cdot ((v_t + \alpha_t)\rho_t)$.

The DOT problem (13) can be seen as a generalized version of DOT with quadratic cost (minimizing a "kinetic energy"); see Eq. (4.41a)-(4.41c) in (Lipman et al., 2024). The GDOT (13) not only minimizes the quadratic cost, but also minimizes the Fisher information and maximizes the expected alignment of the score function with the drift α_t.

In our case, given a pair (Z_0, Z_1) of data points, we are interested in constructing SBs where the marginal constraints are Gaussians centered around Z_0 and Z_1, which we denote as $\xi_0 := \mathcal{N}(Z_0, \sigma_{min}^2 I)$ and $\xi_1 := \mathcal{N}(Z_1, \sigma_{min}^2 I)$ respectively, for some given $\sigma_{min} \geq 0$. These are the Gaussian SBs:

$$\min_{\mathbb{P}_0=\xi_0,\ \mathbb{P}_1=\xi_1} D_{KL}(\mathbb{P}\|\mathbb{Y}). \tag{14}$$

It turns out that the solution of these Gaussian SBs admits a closed-form expression (Bunne et al., 2023).

Theorem 3.2. *The solution $\mathbb{P}^*$ to the Gaussian SB (14) is the path measure of a Markov Gaussian process with the marginal variable $X_t \sim \mathcal{N}(\mu_t, \sigma_t^2 I)$, where*

$$\mu_t = (1 - t + a_t - a_0 - t(a_1 - a_0))Z_0 + (t + b_t - b_0 - t(b_1 - b_0))Z_1, \tag{15}$$

$$\sigma_t^2 = \sigma_{min}^2 + \sigma^2 t(1-t), \tag{16}$$

with $\sigma^2 = \sqrt{4\sigma_{min}^4 + \omega^4} - 2\sigma_{min}^2 > 0$.

See App. D.3 for the proof. In particular, imposing the boundary constraints $a_0 = b_1 = 1, a_1 = b_0 = 0$ on the functions a_t and b_t, we have $\mu_t = a_t Z_0 + b_t Z_1$ in Theorem 3.2. Note that σ_t^2 is independent of a_t and b_t.

3.3 A Novel Probability Path Model

Our proposed probability path model is a stochastic extension of the shortest trajectories connecting consecutive latent samples (Z_0, Z_1), i.e., $\mu_t = (1-t)Z_0 + tZ_1$. Straight trajectories are generally easier to sample with ODE solvers, leading to ODE simulations with smaller errors (Liu et al., 2022). For the stochastic extension, we build on the deterministic backbone and relax the boundary constraints to Gaussians centered around Z_0 and Z_1. We shall look for the "most likely" probability paths connecting the boundary distributions as follows. First, we consider the noise perturbed paths $Z_t = \mu_t + \omega W_t$, where W_t is the standard Wiener process, as our reference process. Then, we take the solution to the Schrödinger bridge (14) with respect to the reference process as our proposed probability path model.

More precisely, in view of Theorem 3.2, we propose to choose $a_t = 1 - t$, $b_t = t$, $c_t^2 = \sigma_{min}^2 + \sigma^2 t(1-t)$, in which case we have the probability path described by:

$$p_t(Z|\tilde{Z}) = \mathcal{N}(Z|tZ_1 + (1-t)Z_0, (\sigma_{min}^2 + \sigma^2 t(1-t))I), \tag{17}$$

which transports a Gaussian distribution centered around Z_0 with variance σ_{min}^2 at $t = 0$ to a Gaussian distribution centered around Z_1 at $t = 1$ with variance σ_{min}^2. Here $\sigma_{min}, \sigma \geq 0$ are tunable parameters. In the case when $\sigma_{min} = 0$, it describes a Brownian bridge that interpolates between Z_0 and Z_1 (Gasbarra et al., 2007). To ensure numerical stability when sampling $t \sim \mathcal{U}[0,1]$, it is beneficial to use a small $\sigma_{min} > 0$. Note that σ^2 is a scale factor determining the magnitude of fluctuations around the path interpolating between

Z_0 and Z_1. The variance c_t^2 is minimum with the value of σ_{min}^2 at the endpoints $t = 0$ and $t = 1$, and the maximum variance is $\sigma_{min}^2 + \sigma^2/4$ which occurs in the middle of the path at $t = 1/2$.

The variance schedule is designed to balance exploration and stability. Low variance at the start ensures stable initialization, preventing the trajectory from deviating too far from the initial distribution. High variance in the middle allows the model to explore diverse paths in the latent space, avoiding mode collapse and enhancing diversity in the generated trajectories. Low variance at the end sharpens the trajectory, ensuring accurate reconstruction of the desired output. This strategy is inspired by findings in diffusion models that utilize a forward noising process and a backward denoising process (Ho et al., 2020; Song et al., 2020b), where such variance patterns have been shown to effectively manage the trade-off between exploration and refinement.

The corresponding VF that defines the flow is then given by (applying Theorem D.2):

$$u_t(Z|\tilde{Z}) = Z_1 - Z_0 + \frac{\sigma^2}{2}\frac{1-2t}{\sigma_{min}^2 + \sigma^2 t(1-t)}\epsilon, \tag{18}$$

where $\epsilon := Z - (tZ_1 + (1-t)Z_0)$. Under reasonable assumptions, the variance of this VF is lower than the variance of the OT-VF of (Lipman et al., 2022) with $\epsilon_{min} := 0$ (rectified flow). Here the variance is taken with respect to the randomness in the samples z^τ and the Gaussian samples drawn during gradient descent updates.

More precisely, denote the VF that corresponds to our model as u_t and the VF that corresponds to the rectified flow model as $\tilde{u}_t$. For a given τ, they generate the probability path $Z_t = tz^\tau + (1-t)z^{\tau-1} + c_t\xi$ and $\tilde{Z}_t = tz^{\tau-1} + (1-t)\eta$ respectively, where $\xi, \eta \sim \mathcal{N}(0, I)$, $c_t = \sqrt{\sigma_{min}^2 + \sigma^2 t(1-t)}$ and $t \in [0, 1]$. Applying Eq. (8), we have:

$$u_t(Z_t|z^{\tau-1}, z^\tau) = z^\tau - z^{\tau-1} + c_t'\xi, \tag{19}$$

$$\tilde{u}_t(\tilde{Z}_t|z^{\tau-1}) = z^{\tau-1} - \eta. \tag{20}$$

Theorem 3.3. *Suppose that $(z^\tau)_{\tau=1,\dots,m}$, with the $z^\tau \in \mathbb{R}^d$, is a discrete-time stochastic process with nonzero correlation in time and let $t \in [0, 1]$ be given. If $Cov(z^{\tau-1}, z^\tau) \geq \frac{1}{2}\left(\left(\frac{\sigma^4}{4\sigma_{min}^2} - 1\right) I + Var(z^\tau)\right)$, then $Var(\tilde{u}_t(\tilde{Z}_t|z^{\tau-1})) \geq Var(u_t(Z_t|z^{\tau-1}, z^\tau))$.*

See App. D.4 for a proof and the related discussions. Theorem 3.3 implies that if the consecutive latent variables z^τ, $z^{\tau-1}$ are sufficiently correlated and σ is chosen small enough relative to σ_{min}, then the variance of the VF that corresponds to our probability path model is lower than that corresponds to the rectified flow model.

4 An Efficient Probabilistic Forecasting Algorithm

In this section, we present efficient algorithms for training and inferencing the flow matching model.

Recently (Davtyan et al., 2023) proposed an efficient algorithm for latent flow matching for the task of video prediction, using the probability path generated by the OT-VF of (Lipman et al., 2022). To enable efficient training, we shall follow (Davtyan et al., 2023) and leverage the iterative nature of sampling from the learned flow and use a single random conditioning element from the past at each iteration. However, our method differs from (Davtyan et al., 2023) as we use different probability paths and target VFs.

Training. Recall that $\tilde{Z} = (Z_0, Z_1)$ denote training samples from $\mathcal{D} = \{(z^{\tau-1}, z^\tau)\}_{\tau=2,\dots,m}$. In other words, we set Z_1 to be the target element and Z_0 to be the reference element chosen to be the previous element before the target element. In this way, our target probability path model maps a distribution centered around a previous state to the distribution of the current states, which is more natural from the point of view of probabilistic forecasting whose goal is to obtain an ensemble of forecasts. Note that this differs from the approach of Davtyan et al. (2023), where $\tilde{Z} = Z_1$ (i.e., they do not use a reference element to define their probability path, whereas we use a pair of elements (Z_0, Z_1)). Algorithm 1 summarizes the training procedure of our method.

Both the autoencoder and the VF neural network can also be jointly trained in an end-to-end manner, but our empirical results show that separating the training can lead to improved performance. Moreover, doing so allows us to better assess the impact of using different probability paths.

Algorithm 1 Flow matching for spatio-temporal data

Input: Dataset of sequences D, number of iterations M
for i in range(1, M) **do**
  Sample a sequence $\mathbf{x}$ from the dataset D
  Encode it with a pre-trained encoder to obtain $\mathbf{z}$
  Choose a random target element $z^\tau, \tau \in \{3, \dots |\mathbf{z}|\}$, from $\mathbf{z}$
  Sample a step $t \sim U[0, 1]$
  Sample a noisy observation $Z \sim p_t(Z \mid z^\tau, z^{\tau-1})$, where p_t is given by Eq. (7)
  Compute $u_t(Z \mid z^\tau, z^{\tau-1})$
  Sample a condition frame $z^c, c \in \{1, \dots \tau - 2\}$
  Update the parameters θ via gradient descent

$$\nabla_\theta \| v_t^\theta(Z \mid z^{\tau-1}, z^c, \tau - c) - u_t(Z \mid z^\tau, z^{\tau-1}) \|^2$$

end for
Return: A learned VF, $v_t^{\theta^*}$

Inference. We use an ODE sampler during inference to generate forecasts. The ODE sampler is described as follows. Let $(Y_i^\tau)_{i=0,\dots,N}$ denote the generation process, where N is the number of integration steps and the superscript τ denotes the time index for which the generation/forecast is intended for. Given the previous elements $(x^1, \dots, x^{T-1})$ of a time series sample, in order to generate the next element (i.e., the T-th element), we start with sampling the initial condition Y_0^T from $\mathcal{N}(z^{T-1}, \sigma_{sam}^2 I)$ for some small $\sigma_{sam} \geq 0$, where $z^{T-1} = \mathcal{E}(x^{T-1})$. This is in contrast to the procedure of (Davtyan et al., 2023), which simply uses a mean-zero Gaussian sample instead. We then use an ODE solver to integrate the learned VF along the time interval $[0, 1]$ to obtain Y_N^T. We use $\mathcal{D}(Y_N^T)$ as an estimate of x^T, and forecasting is done autoregressively. Algorithm 2 summarizes this procedure when the sampling is done using the forward Euler scheme. Note that we can also use computationally more expensive numerical schemes such as the Runge-Kutta (RK) schemes.

Algorithm 2 One-step ahead forecasting with forward Euler

Input: A sequence $(x^1, \dots, x^{T-1})$ containing the previous elements, number of integration steps N, grid $s_0 = 0 < s_1 < \dots < s_N = 1$, a learnt VF $v_s^{\theta^*}$ for $s \in [0, 1]$
Set $\Delta s_n = s_{n+1} - s_n$ for $n = 0, \dots, N-1$
Sample $Y_0^T \sim \mathcal{N}(\mathcal{E}(x^{T-1}), \sigma_{sam}^2 I)$, $\sigma_{sam} \geq 0$
for n in range(0, $N-1$) **do**
  Sample $c \sim \mathcal{U}(2, \dots, T-1)$
  $y^{T-c} = \mathcal{E}(x^{T-c})$
  $Y_{n+1}^T = Y_n^T + \Delta s_n v_{s_n}^{\theta^*}(Y_n^T | Y_0^T, y^{T-c}, T-c)$
end for
Return: An estimate of x^T, $\hat{x}^T = \mathcal{D}(Y_N^T)$

5 Empirical Results

In this section, we present our main empirical results to elucidate the design choice of probability paths within the flow matching framework (comparison with other generative modeling frameworks is not our focus here). We focus on PDE dynamics forecasting tasks here (additional details and results can be found in App. E-F). We test the performance of our probability path model, i.e., Eq. (17) with $a_t = 1 - t$, $b_t = t$ and $c_t = \sqrt{\sigma_{min}^2 + \sigma^2 t(1-t)}$ on these tasks. We pick $\sigma_{min} = 0.001$, and treat σ and σ_{sam} as tunable parameters. We compare our proposed model with four other models of probability paths:

- **RIVER** (Davtyan et al., 2023): RIVER uses the OT-VF model in Table 1, i.e., $a_t = 0$, $b_t = t$, $c_t = 1 - (1 - \epsilon_{min})t$, choosing $\epsilon_{min} = 10^{-7}$.
- **VE-diffusion** in Table 1: We use $\sigma_t = \sigma_{min}\sqrt{\left(\frac{\sigma_{max}}{\sigma_{min}}\right)^{2t} - 1}$ with $\sigma_{min} = 0.01$, $\sigma_{max} = 0.1$, and sample t uniformly from $[0, 1 - \epsilon]$ with $\epsilon = 10^{-5}$ following (Song et al., 2020b).
- **VP-diffusion** in Table 1: We use $\beta(s) = \beta_{min} + s(\beta_{max} - \beta_{min})$ where $\beta_{min} = 0.1, \beta_{max} = 20$ and t is sampled from $\mathcal{U}[0, 1 - \epsilon]$ with $\epsilon = 10^{-5}$, following (Song et al., 2020b). Thus, $T(s) = s\beta_{min} + \frac{1}{2}s^2(\beta_{max} - \beta_{min})$.
- **The stochastic interpolant (SI) path** in Table 1: We consider the path proposed by (Chen et al., 2024) and use the suggested choice of $a_t = 1 - t$, $b_t = t^2$ and $c_t = \epsilon(1 - t)\sqrt{t}$ (see Eq. (2) in (Chen et al., 2024) and note that $Var((1 - t)W_t) = (1 - t)^2 t$ for the standard Wiener process W_t). We choose $\epsilon = 0.01$. This is a path that is similar to ours, but with the variance c_t^2 chosen such that the maximum occurs at $t = 1/\sqrt{3}$ instead of at the middle of the path at $t = 1/2$. Later, we will see that different forms of variance can lead to vastly different performance in the considered tasks.

Evaluation metrics. We evaluate the models using the following metrics. First, we use the standard mean squared error (MSE) and the relative Frobenius norm error (RFNE) to measure the difference between predicted and true snapshots. Second, we compute metrics such as the peak signal-to-noise ratio (PSNR), and the structural similarity index measure (SSIM) to further quantify the quality and similarity of the generated snapshots (Wang et al., 2004). Third, we use the Pearson correlation coefficient to assess the correlation between predicted and true snapshots.

Training details. We use an autoencoder (AE) to embed the training data into a low-dimensional latent space, which enables the model to capture the most relevant features of the data while reducing dimensionality (Azencot et al., 2020); see App. F for further discussion of the motivation. We then train a flow matching model in this latent space. Training generative models in latent space has also been considered by (Vahdat et al., 2021) for score matching models and by (Dao et al., 2023) for flow matching models. To train the AE, we minimize a loss function that consists of reconstruction error, in terms of MSE, between the input data and its reconstructed version from the latent space. The choice of the AE architecture is tailored to the complexity of the dataset (see App. F for details).

5.1 Probabilistic Forecasting of Dynamical Systems

We evaluate the performance of our proposed probability path model on challenging dynamical systems to demonstrate its effectiveness in forecasting complex continuous dynamics. Specifically, we consider the following tasks (for details see App. F.1):

- **Fluid Flow Past a Cylinder (FPC):** This task involves forecasting the vorticity of a fluid flowing past a cylinder. The model conditions on the first 5 frames and predicts the subsequent 20 frames at a resolution of 64×64 with 1 channel representing vorticity.
- **Shallow-Water Equation (SWE):** This dataset models the dynamics of shallow-water equations (Takamoto et al., 2022), capturing essential aspects of geophysical fluid flows. We use the first 5 frames for conditioning and predict the next 15 frames at a resolution of 128×128 with 1 channel representing horizontal flow velocity.
- **Diffusion-Reaction Equation (DRE):** This dataset models the dynamics of a 2D diffusion-reaction equation (Takamoto et al., 2022). We use the first 5 frames for conditioning and predict 15 future frames at a 128×128 with 2 channels representing velocity in the x and y directions.
- **Incompressible Navier-Stokes Equation (NSE):** As a more challenging benchmark, we consider forecasting the dynamics of a 2D incompressible Navier-Stokes equation (Takamoto et al., 2022). We use the first 5 frames for conditioning and predict the next 20 frames at a resolution of 512×512 with 2 channels representing velocity in the x and y directions.

Table 2 summarizes the performance of our model compared to other probability path models across all tasks. It can be seen that our probability path model achieves the lowest test MSE and RFNE across all tasks, indicating more accurate forecasts. Moreover, the higher PSNR and SSIM scores indicate that our model better preserves spatial structures in the predictions. Despite the similarity of our proposed model with the stochastic interpolant of (Chen et al., 2024), in that both models use consecutive samples to define the path, our model outperforms the stochastic interpolant model, suggesting that choosing the maximum variance to occur at the middle of the path is a better choice. Importantly, our model is highly efficient during inference time since it requires only 10 sampling steps; this is significantly fewer than the 50 steps needed by other models.

Figure 1 shows the Pearson correlation coefficients of the predicted snapshots over time for all models. Our model's predictions shows a slower decay of correlation coefficients compared to other models, indicating better temporal consistency and long-term predictive capability. Correlation coefficients about 95% indicate performance on par with physics-based numerical simulators.

Table 2: Results for forecasting dynamical systems using different probability path models for flow matching. Results are averaged over 5 generations obtained with 10 sampling steps using RK4.

Task	Model	Test MSE (↓)	Test RFNE (↓)	PSNR (↑)	SSIM (↑)
Flow past Cylinder	RIVER	3.05e-03	5.70e-02	42.66	0.98
	VE-diffusion	2.75e-01	5.21e-01	26.81	0.52
	VP-diffusion	3.20e-03	5.20e-01	42.60	0.97
	Stochastic interpolant	3.39e-03	6.09e-02	41.82	0.97
	Ours	**3.80e-04**	**2.30e-02**	**48.89**	**0.99**
Shallow-Water	RIVER	9.29e-04	1.5e-01	34.90	0.91
	VE-diffusion	1.23e-02	5.5e-01	28.76	0.57
	VP-diffusion	1.31e-03	1.8e-01	34.33	0.88
	Stochastic interpolant	1.06e-03	1.5e-01	35.57	0.88
	Ours	**6.90e-04**	**1.3e-01**	**36.10**	**0.93**
Diffusion-Reaction	RIVER	2.37e-03	2.07e-01	38.47	0.84
	VE-diffusion	9.74e-02	1.7	32.83	0.35
	VP-diffusion	1.72e-02	6.48e-01	34.65	0.53
	Stochastic interpolant	6.17e-02	8.62e-01	**45.64**	0.76
	Ours	**3.56e-04**	**1.16e-01**	34.34	**0.89**
Navier-Stokes	RIVER	1.98e-04	2.5e-01	38.71	0.85
	VE-diffusion	1.21e-04	2.4	29.53	0.27
	VP-diffusion	7.62e-02	1.85e-01	40.73	0.93
	Stochastic interpolant	7.26e-05	1.8e-01	37.81	0.88
	Ours	**1.90e-05**	**9.8e-02**	**41.52**	**0.96**

Figure 3 (see App. F) compares the training loss curves of our model with others for the FPC and the SWE task. Our method leads to faster convergence during training and smoother loss curves. This suggests that our model requires fewer iterations to generate high-quality samples when compared to other models.

5.2 Discussion

Our empirical results showed that our proposed model consistently outperformed other models across several forecasting tasks involving different PDEs. Our model shows improved training efficiency, with faster convergence reducing the computational resources and time required for model training. Moreover, our model is efficient during inference time since it only requires a few sampling steps, making it practical for real-world applications where computational efficiency is crucial. Additionally, the model maintained better temporal consistency, as indicated by a slower decay of Pearson correlation coefficients over longer prediction horizons. These findings validate the effectiveness of our approach in modeling complex dynamical systems.

Our ablation study (see App. E.2) further validated the advantages of our proposed probability path model. We found that larger σ values not only contributed to smoother training loss curves but also enhanced the overall stability and efficiency of the model. Moreover, we saw that $\sigma_{\text{sam}} = 0$ can be fixed without

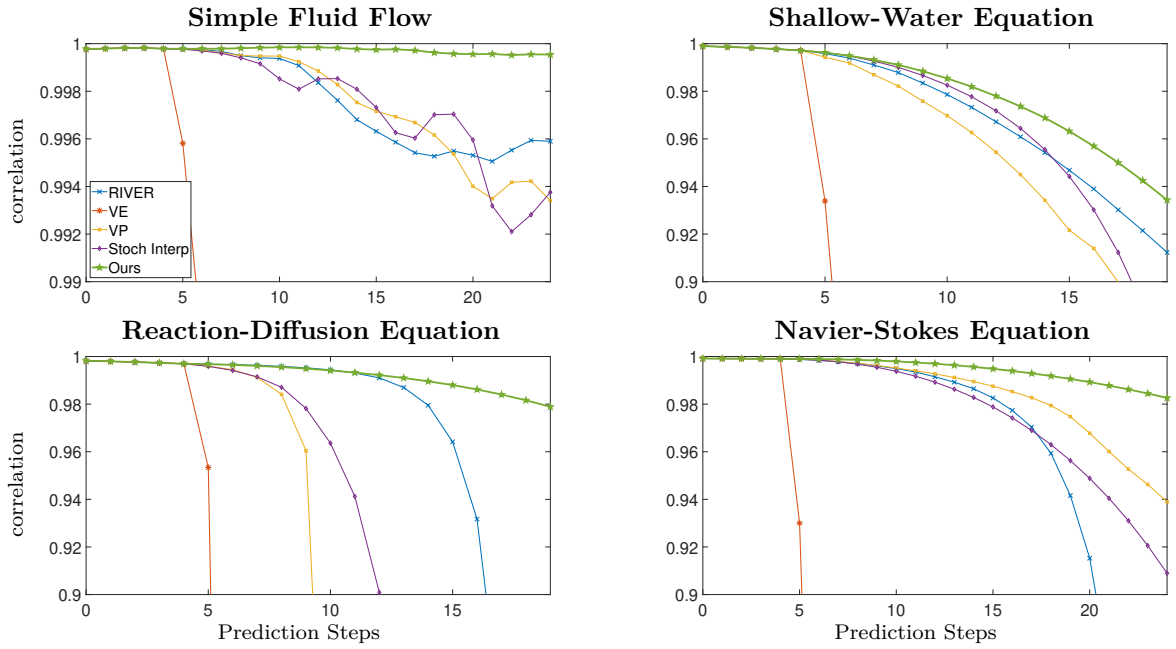

Figure 1: Pearson correlation coefficient to assess the correlation between predicted and true snapshots at various prediction steps for different probability path models. Our probability path model shows the best performance on all three tasks. Note that the first 5 snapshots are the conditioning snapshots.

compromising accuracy. The fact that our model achieved improved performance even with the simplest sampler (Euler scheme) and a minimal number of sampling steps (as few as five) validates its practical applicability, especially in scenarios where computational resources and time are limited.

6 Conclusion

In this work, we investigated the use of flow matching in latent space for probabilistic forecasting of spatio-temporal dynamics, providing a theoretical framework and efficient algorithms. We demystified the critical role of the probability path design in this setting and proposed an improved probability path model. Our model is theoretically motivated via the SB and dynamical optimal transport perspective. It leverages the inherent continuity and correlation in the spatio-temporal data, leading to more stable training and faster convergence. Our empirical evaluations on several PDE forecasting tasks demonstrated that our model performs favorably when compared to existing models. While we focus on the flow matching approach here, we leave comprehensive comparisons with other approaches such as score matching and bridge matching to future work.

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Appendix

This appendix is organized as follows. In App. A, we provide a detailed discussion of related work and connect them to our studies. In App. B, we provide some remarks on the connection of flow matching models to other generative models. In App. C, we provide commonly used loss parametrizations and compare them with our flow matching loss. In App. D, we provide theorems and proofs to justify the discussions in Section 2-3 (see Theorem D.1-D.2 and Theorem 3.2-3.3), as well as additional discussions. In App. E, we provide additional empirical results. In App. F, we provide the missing experimental details.

A Related Work

Modeling and forecasting dynamical systems. Traditionally dynamical systems arising in scientific applications have been studied through mathematical models based on physical laws, such as ODEs and PDEs (Evans, 2022). These methods often require significant domain knowledge and strong assumptions, limiting their flexibility in data-driven scenarios where governing equations are unknown. Statistical and machine learning (ML) methods have emerged as powerful alternatives to study these systems. Classical approaches include autoregressive integrated moving average (ARMA) and state-space models such as Kalman filters (Box et al., 2015), which have long been used for time series forecasting but struggle with highly nonlinear dynamics. ML methods such as recurrent neural networks (RNNs) (Bengio et al., 2013) and variants for spatio-temporal data (Shi et al., 2015; Lyu et al., 2024) are capable of learning complex temporal dependencies but they are challenging to train. Neural ODEs (Chen et al., 2018; Queiruga et al., 2021) offer a structured approach to continuous-time modeling by integrating neural networks with ODE solvers. However, these models still face challenges with generalizing to new systems, and learning continuous physical dynamics (Krishnapriyan et al., 2023).

Generative modeling for time series forecasting. Generative models, particularly score-based diffusion models and flow-based approaches, have gained significant attention for learning complex data distributions in high-dimensional spaces such as images (Song et al., 2020b; Karras et al., 2022; Esser et al., 2024), videos (Davtyan et al., 2023; Shrivastava & Shrivastava, 2024), and dynamical systems (Pathak et al., 2024; Kohl et al., 2024; Ren et al., 2024). In the context of time series forecasting, diffusion models like TimeGrad (Rasul et al., 2021; Meijer & Chen, 2024) incorporate conditioning on previous time steps into both the forecasting process and the loss function. Building upon TimeGrad, CSDI (Tashiro et al., 2021) enhances performance in imputation tasks by replacing the RNN encoder with a transformer. ScoreGrad (Yan et al., 2021) adapts this framework to a score-based diffusion model for multivariate probabilistic forecasting. Methods such as DSPD and CSPD (Biloš et al., 2023), based on DDPM and SDE respectively, model dynamics as continuous functions and introduce time-correlated noise functions. Another relevant work, SSSD^{S4} (Alcaraz & Strodthoff, 2023), uses state-space models (S4) to encode time series and performs diffusion over the temporal domain instead of across multivariate components. While these models demonstrate strong performance, they often require many sampling steps during generation. Related to our approach, (Chen et al., 2024) proposes an SDE framework utilizing stochastic interpolants (Albergo et al., 2023) for probabilistic forecasting, but their sampler also requires many steps during generation. Another recent work is (Tamir et al., 2024), which introduces a flow matching framework for time series modeling within the data space; however, it concentrates on small ODE datasets and does not address forecasting tasks.

Applications of diffusion models to spatio-temporal data have primarily focused on video generation (Singer et al., 2023). For spatio-temporal forecasting on sensor grids, graph neural networks (GNNs) are widely employed in tasks such as traffic prediction (Qu et al., 2023; Lv et al., 2024; Wen et al., 2024) and air quality forecasting (Wen et al., 2024). Another recent work is DYffusion (Cachay et al., 2023), which utilizes a non-Markovian diffusion process to propagate images temporally, similar to DDIM. This method iteratively refines initial predictions at larger time steps by conditioning them on predictions at smaller time steps.

B Connection to SDE Based Generative Model Frameworks

In this section, we provide some remarks on the connection between flow matching models and SDE based generative models (Song et al., 2020b).

Consider the following continuous-time Gaussian latent variable model (Tomczak, 2021): $Z_t = \mathcal{E}(X_t)$,

$$Z_t = A_t Z_0 + B_t Z_1 + L_t \epsilon, \quad t \in [0,1], \tag{21}$$

$$X_t = \mathcal{D}(Z_t), \tag{22}$$

where t is the continuous variable, $X_0 \in \mathbb{R}^d$ represent data samples, $Z \in \mathbb{R}^p$ is the latent variable, $\epsilon \sim \mathcal{N}(0, I)$ is independent of the random variables X_0, Z_0, Z_1. Here A_t, B_t and $L_t \geq 0$ are pre-specified coefficients which are possibly matrix-valued and time-dependent, $\mathcal{D}$ and $\mathcal{E}$ denote the decoder and encoder map respectively, and $\mathcal{D} \circ \mathcal{E} = I$. Note that Z_0 and Z_1 are initial and terminal point of the path $(Z_t)_{t\in[0,1]}$ in the latent space.

The above latent variable model can be identified (up to equivalence in law for each t) with the linear SDE of the form:

$$d\hat{Z}_t = F_t \hat{Z}_t dt + H_t Z_1 dt + G_t dW_t, \quad \hat{Z}_0 = Z_0, \quad t \in [0,1), \tag{23}$$

where $(W_t)_{t\in[0,1]}$ is the standard Wiener process. By matching the moments, we obtain

$$F_t = \dot{A}_t A_t^{-1}, \tag{24}$$

$$H_t = \dot{B}_t - \dot{A}_t A_t^{-1} B_t, \tag{25}$$

$$G_t G_t^T = \dot{L}_t L_t^T + L_t \dot{L}_t^T - \dot{A}_t A_t^{-1} L_t L_t^T - L_t L_t^T A_t^{-T} (\dot{A}_t)^T, \tag{26}$$

where the overdot denotes derivative with respect to t and A^T denotes the transpose of A.

Under the above formulation, various existing generative models such as DDPM (Ho et al., 2020), VP-SDE and VE-SDE of (Song et al., 2020b;a), the critically damped SDE of (Dockhorn et al., 2021), the flow matching models in (Lipman et al., 2022; Tong et al., 2023b; Liu et al., 2022) and the stochastic interpolants of (Albergo et al., 2023) can be recovered, and new models can be derived.

The following proposition establishes the connection between flow matching using our proposed probability path model, the Gaussian latent variable model (21) and the linear SDE model (23).

Proposition B.1. *For every $t \in [0,1]$, the Z_t defined in Eq. (17) can be identified, up to equivalence in law, with the Z_t generated by the latent variable model (21) with $A_t = (1-t)I$, $B_t = tI$, $L_t = \sqrt{\sigma_{min}^2 + \sigma^2 t(1-t)}I$. For $t \in [0,1)$, it can also be identified with the solution $\hat{Z}_t$ of the linear SDE (23) with $F_t = -I/(1-t)$, $H_t = (1 + \frac{t}{1-t})I$ and $G_t = \sqrt{\sigma^2 + \frac{2\sigma_{min}^2}{1-t}}I$. Moreover, $\lim_{t\to 1} \hat{Z}_t =^d Z_1 + \sigma_{min}\epsilon$, where $\epsilon \sim \mathcal{N}(0, I)$ and $=^d$ denotes equivalence in distribution.*

Proof. The identification follows from matching the moments of Z_t and $\hat{Z}_t$, i.e., applying Eq. (24)-(26).

To prove that $\lim_{t\to 1} \hat{Z}_t =^d Z_1 + \sigma_{min}\epsilon$, we use the explicit solution of the SDE:

$$\hat{Z}_t = \Phi(t,0)Z_0 + \int_0^t \Phi(t,s) H_s Z_1 ds + \int_0^t \Phi(t,s) G_s dW_s,$$

where $\Phi(t,s)$ is the fundamental solution of the homogeneous equation $d\Phi(t,s) = F_t \Phi(t,s)dt$ with $\Phi(s,s) = I$. For our $F_t = -I/(1-t)$, we have $\Phi(t,s) = \exp(-\int_s^t \frac{1}{1-u}du)I = (\frac{1-t}{1-s})I$. Substituting this and the formula for H_t into the solution, we obtain $\hat{Z}_t = (1-t)Z_0 + \int_0^t (\frac{1-t}{1-s})(1 + \frac{s}{1-s})Z_1 ds + \int_0^t (\frac{1-t}{1-s})\sqrt{\sigma^2 + \frac{2\sigma_{min}^2}{1-s}} I dW_s$.

Now, let us examine each term as $t \to 1$. First, $(1-t)Z_0 \to 0$ as $t \to 1$ and $\int_0^t (\frac{1-t}{1-s})(1 + \frac{s}{1-s})Z_1 ds = tZ_1 \to Z_1$ as $t \to 1$. It remains to deal with the stochastic integral term $M_t := \int_0^t (\frac{1-t}{1-s})\sqrt{\sigma^2 + \frac{2\sigma_{min}^2}{1-s}} dW_s$. Note that

M_t is an Itô integral that has zero mean, i.e. $\mathbb{E}M_t = 0$, and using Itô's formula (Särkkä & Solin, 2019),

$$\mathbb{E}M_t^2 = \int_0^t ((1-t)/(1-s))^2 \left(\sigma^2 + \frac{2\sigma_{min}^2}{1-s}\right) ds \tag{27}$$

$$= (1-t)^2 \left[\sigma^2 \int_0^t \frac{1}{(1-s)^2} ds + 2\sigma_{min}^2 \int_0^t \frac{1}{(1-s)^3} ds\right] \tag{28}$$

$$= (1-t)^2 \left[\sigma^2 \left(\frac{t}{1-t}\right) + \sigma_{min}^2 \left(\frac{1}{(1-t)^2} - 1\right)\right] \tag{29}$$

$$= (1-t)t\sigma^2 + \sigma_{min}^2 t(2-t), \tag{30}$$

which tends to σ_{min}^2 as $t \to 1$. Combining the above results, $\lim_{t\to 1} \hat{Z}_t \sim \mathcal{N}(Z_1, \sigma_{min}^2 I)$.

□

C On Different Loss Parametrizations

In this section, we list popular choices of loss parametrization considered in the literature and connect them to our flow matching loss. We refer to (Kingma & Gao, 2023) for a more comprehensive discussion. Recall that the Gaussian path that we consider is: $Z_t = a_t Z_0 + b_t Z_1 + c_t \xi$, where $\xi \sim \mathcal{N}(0, I)$. In general, these loss parametrizations take the form of:

$$\mathcal{L}(\theta) := \mathbb{E}_{t, p_t(Z|\tilde{Z}), q(\tilde{Z})} \omega(t) \| m_t^\theta(Z) - m_t(Z, \tilde{Z}) \|^2, \tag{31}$$

where $\omega(t) > 0$ is a weighting function, $m_t(Z, \tilde{Z})$ is the object (conditioned on $\tilde{Z}$) to be learnt and m_t^θ is a neural network model used to learn the object of interest. Depending on which object one would like to learn/match, we have different loss parametrizations.

Flow matching. The flow matching loss that we focus in this paper is:

$$\mathcal{L}_{cfm}(\theta) := \mathbb{E}_{t, p_t(Z|\tilde{Z}), q(\tilde{Z})} \omega(t) \| v_t^\theta(Z) - u_t(Z|\tilde{Z}) \|^2, \tag{32}$$

where one aims to learn the flow generating vector field:

$$u_t(Z|\tilde{Z}) = \frac{c_t'}{c_t}(Z - (a_t Z_0 + b_t Z_1)) + a_t' Z_0 + b_t' Z_1, \tag{33}$$

Score matching. The score matching loss is:

$$\mathcal{L}_{sm}(\theta) := \mathbb{E}_{t, p_t(Z|\tilde{Z}), q(\tilde{Z})} \lambda(t) \| s_t^\theta(Z) - \nabla \log p_t(Z|\tilde{Z}) \|^2, \tag{34}$$

where $\lambda(t) > 0$ is a weighting function and one aims to learn the score function:

$$\nabla \log p_t(Z|\tilde{Z}) = \frac{a_t Z_0 + b_t Z_1 - Z}{c_t^2}. \tag{35}$$

If $\lambda(t) = c_t^2$, then this reduces to the original score matching loss (Song & Ermon, 2019), whereas if $\lambda(t) = \beta(1-t)$, this becomes the score flow loss (Song et al., 2021).

Noise matching. The noise matching loss is:

$$\mathcal{L}_{nm}(\theta) := \mathbb{E}_{t, p_t(Z|\tilde{Z}), q(\tilde{Z})} \| \epsilon_t^\theta(Z) - \epsilon_t(Z|\tilde{Z}) \|^2, \tag{36}$$

where one aims to learn the noise:

$$\epsilon_t(Z|\tilde{Z}) = \frac{Z - (a_t Z_0 + b_t Z_1)}{c_t}. \tag{37}$$

D Theoretical Results and Proofs

In this section, we provide theorems and proofs to justify the discussions in Section 2 and Section 3.

D.1 Connecting Flow Matching with Conditional Flow Matching

The following theorem justifies the claim that minimizing $\mathcal{L}_{fm}$ is equivalent to minimizing $\mathcal{L}_{cfm}$.

Theorem D.1. *If the conditional vector field $u_t(Z|\tilde{Z})$ generates the conditional probability path $p_t(Z|\tilde{Z})$, then the marginal vector field u_t in Eq. (5) generates the marginal probability path p_t in Eq. (4). Moreover, if $p_t(Z) > 0$ for all t, Z, then $\mathcal{L}_{fm}$ and $\mathcal{L}_{cfm}$ are equal up to a constant independent of θ.*

Proof. The proof is a straightforward extension of the proofs of Theorem 1-2 in (Lipman et al., 2022) from conditioning on data samples to conditioning on latent samples and allowing an arbitrary weighting function $\omega(t)$.

Suppose that the conditional vector field $u_t(Z|\tilde{Z})$ generates the conditional probability path $p_t(Z|\tilde{Z})$, we would like to show that the marginal vector field u_t in Eq. (5) generates the marginal probability path p_t in Eq. (4). To show this, it suffices to verify that p_t and u_t satisfy the continuity equation:

$$\frac{d}{dt}p_t(Z) + div(p_t(Z)u_t(Z)) = 0, \tag{38}$$

where the divergence operator, div, is defined with respect to the latent variable $Z = (Z^1, \ldots, Z^d)$, i.e., $div = \sum_{i=1}^{d} \frac{\partial}{\partial Z^i}$.

We begin by taking derivative of $p_t(Z)$ with respect to time:

$$\begin{aligned}
\frac{d}{dt}p_t(Z) &= \frac{d}{dt}\int p_t(Z|\tilde{Z})q(\tilde{Z})d\tilde{Z} && (39)\\
&= \int \frac{d}{dt}p_t(Z|\tilde{Z})q(\tilde{Z})d\tilde{Z} && (40)\\
&= -\int div(u_t(Z|\tilde{Z})p_t(Z|\tilde{Z}))q(\tilde{Z})d\tilde{Z} && (41)\\
&= -div\left(\int u_t(Z|\tilde{Z})p_t(Z|\tilde{Z})q(\tilde{Z})d\tilde{Z}\right) && (42)\\
&= -div(u_t(Z)p_t(Z)). && (43)
\end{aligned}$$

In the third line, we use the fact that $u_t(\cdot|\tilde{Z})$ generates $p_t(\cdot|\tilde{Z})$. In the last line, we use Eq. (5). In the second and forth line above, the exchange of integration and differentiation can be justified by assuming that the integrands satisfy the regularity conditions of the Leibniz rule.

Next, we would like to show that if $p_t(Z) > 0$ for all t, Z, then $\mathcal{L}_{fm}$ and $\mathcal{L}_{cfm}$ are equal up to a constant independent of θ. We follow (Lipman et al., 2022) and assume that $q(Z)$ and $p_t(Z|\tilde{Z})$ are decreasing to zero sufficiently fast as $\|Z\| \to 0$, that $u_t, v_t, \nabla_\theta v_t$ are bounded, so that all integrals exist and exchange of integration order is justified via Fubini's theorem.

Using the bilinearity of the 2-norm, we decompose the squared losses as:

$$\|v_t^\theta(Z) - u_t(Z)\|^2 = \|v_t^\theta(Z)\|^2 - 2\langle v_t^\theta(Z), u_t(Z)\rangle + \|u_t(Z)\|^2, \tag{44}$$

$$\|v_t^\theta(Z) - u_t(Z|\tilde{Z})\|^2 = \|v_t^\theta(Z)\|^2 - 2\langle v_t^\theta(Z), u_t(Z|\tilde{Z})\rangle + \|u_t(Z|\tilde{Z})\|^2. \tag{45}$$

Now,

$$\mathbb{E}_{p_t(Z)}\|v_t^\theta(Z)\|^2 = \int \|v_t^\theta(Z)\|^2 p_t(Z)dZ \tag{46}$$

$$= \int\int \|v_t^\theta(Z)\|^2 p_t(Z|\tilde{Z})q(\tilde{Z})d\tilde{Z}dZ \tag{47}$$

$$= \mathbb{E}_{q(\tilde{Z}),p_t(Z|\tilde{Z})}\|v_t^\theta(Z)\|^2, \tag{48}$$

where we use Eq. (4) in the second equality above and exchange the order of integration in the third equality.

Next, we compute:

$$\mathbb{E}_{p_t(Z)}\langle v_t^\theta(Z), u_t(Z)\rangle = \int \left\langle v_t^\theta(Z), \frac{\int u_t(Z|\tilde{Z})p_t(Z|\tilde{Z})q(\tilde{Z})d\tilde{Z}}{p_t(Z)}\right\rangle p_t(Z)dZ \tag{49}$$

$$= \int \left\langle v_t^\theta(Z), \int u_t(Z|\tilde{Z})p_t(Z|\tilde{Z})q(\tilde{Z})d\tilde{Z}\right\rangle dZ \tag{50}$$

$$= \int\int \langle v_t^\theta(Z), u_t(Z|\tilde{Z})\rangle p_t(Z|\tilde{Z})q(\tilde{Z})d\tilde{Z}dZ \tag{51}$$

$$= \mathbb{E}_{q(\tilde{Z}),p_t(Z|\tilde{Z})}\langle v_t^\theta(Z), u_t(Z|\tilde{Z}), \tag{52}$$

where we first plug in Eq. (5) and then exchange the order the integration in order to arrive at the last equality.

Finally, noting that u_t are $\omega(t)$ independent of θ (and are thus irrelevant for computing the loss gradients), we have proved the desired result. □

D.2 Identifying the Vector Field that Generates the Gaussian Paths

Similar to Theorem 3 in (Lipman et al., 2022), we have the following result, which identifies the unique vector field that generates the Gaussian probability path.

Theorem D.2. *Let $p_t(Z|\tilde{Z})$ be the Gaussian probability path defined in Eq. (7) and consider the flow map ψ_t defined as $\psi_t(Z) = a_tZ_0 + b_tZ_1 + c_tZ$ with $c_t > 0$. Then the unique vector field that defines ψ_t is:*

$$u_t(Z|\tilde{Z}) = \frac{c_t'}{c_t}(Z - (a_tZ_0 + b_tZ_1)) + a_t'Z_0 + b_t'Z_1, \tag{53}$$

where prime denotes derivative with respect to t, and $u_t(Z|\tilde{Z})$ generates the Gaussian path $p_t(Z|\tilde{Z})$.

Proof. Let $p_t(Z|\tilde{Z})$ be the Gaussian probability path defined in Eq. (7) and consider the flow map ψ_t defined as $\psi_t(Z) = a_tZ_0 + b_tZ_1 + c_tZ$. We would like to show that the unique vector field that defines ψ_t is:

$$u_t(Z|\tilde{Z}) = \frac{c_t'}{c_t}(Z - (a_tZ_0 + b_tZ_1)) + a_t'Z_0 + b_t'Z_1, \tag{54}$$

and $u_t(Z|\tilde{Z})$ generates the Gaussian path $p_t(Z|\tilde{Z})$.

We denote $w_t = u_t(Z|\tilde{Z})$ for notational simplicity. Then,

$$\frac{d}{dt}\psi_t(Z) = w_t(\psi_t(Z)). \tag{55}$$

Since ψ_t is invertible (as $c_t > 0$), we let $Z = \psi^{-1}(Y)$ and obtain

$$\psi_t'(\psi^{-1}(Y)) = w_t(Y), \tag{56}$$

where the prime denotes derivative with respect to t and we have used the apostrosphe notation for the derivative to indicate that ψ_t' is evaluated at $\psi^{-1}(Y)$.

Inverting $\psi_t(Z)$ gives:

$$\psi_t^{-1}(Y) = \frac{Y - \mu_t(\tilde{Z})}{c_t}, \tag{57}$$

where $\mu_t(\tilde{Z}) := a_t Z_0 + b_t Z_1$.

Differentiating ψ_t with respect to t gives $\psi_t'(Z) = c_t' Z + \mu_t'(\tilde{Z})$.

Plugging the last two equations into Eq. (56), we obtain:

$$w_t(Y) = \frac{c_t'}{c_t}(Y - \mu_t(\tilde{Z})) + \mu_t'(\tilde{Z}) \tag{58}$$

which is the result that we wanted to show.

□

D.3 Solution to the Gaussian Schrodinger Bridge Problem

We prove Theorem 3.2 in this subsection. First, we recall Theorem 3 from (Bunne et al., 2023). Theorem 3.2 then follows from an application of the theorem.

Let $\xi_0 \sim \mathcal{N}(\mu_0, \Sigma_0)$ and $\xi_1 \sim \mathcal{N}(\mu_1, \Sigma_1)$ be two given Gaussian random variables. From now on, by abusing the notation we will also denote the measures of these Gaussians by ξ_0 and ξ_1 respectively.

Let $\sigma \geq 0$ and set:

$$D_\sigma := (4\Sigma_0^{1/2}\Sigma_1\Sigma_0^{1/2} + \sigma^4 I)^{1/2} \tag{59}$$

$$C_\sigma := \frac{1}{2}(\Sigma_0^{1/2} D_\sigma \Sigma_0^{-1/2} - \sigma^2 I). \tag{60}$$

Consider the following Schrodinger bridges with Gaussian marginal constraints:

$$\min_{\mathbb{P}_0 = \xi_0, \mathbb{P}_1 = \xi_1} D_{KL}(\mathbb{P} \| \mathbb{Q}), \tag{61}$$

where $\mathbb{Q}$ is the path measure of the linear SDE:

$$dY_t = (c_t Y_t + \alpha_t)dt + g_t dW_t := f_t dt + g_t dW_t. \tag{62}$$

Here, $c_t : \mathbb{R}^+ \to \mathbb{R}$, $\alpha_t : \mathbb{R}^+ \to \mathbb{R}^d$ and $g_t : \mathbb{R}^+ \to \mathbb{R}^+$ are smooth functions, and W_t is the standard Wiener process.

The following theorem is a simplified version of Theorem 3 in (Bunne et al., 2023).

Theorem D.3 (Theorem 3 in (Bunne et al., 2023))**.** *The solution $\mathbb{P}^*$ to the Gaussian Schrodinger bridges is (the path measure of) a Markov Gaussian process whose marginal variable $X_t \sim \mathcal{N}(\mu_t, \Sigma_t)$, where*

$$\mu_t = (\tau_t - r_t\tau_1)\mu_0 + r_t\mu_1 + \zeta(t) - r_t\zeta(1), \tag{63}$$

$$\Sigma_t = (\tau_t - r_t\tau_1)^2\Sigma_0 + r_t^2\Sigma_1 + r_t(\tau_t - r_t\tau_1)(C_{\sigma^*} + C_{\sigma^*}^T) + \kappa(t,t)(1-\rho_t)I. \tag{64}$$

In the above,

$$\tau_t = \exp\left(\int_0^t c_s ds\right), \quad \kappa(t,t') = \tau_t\tau_{t'}\int_0^t \tau_s^{-2} g_s^2 ds, \quad r_t = \kappa(t,1)/\kappa(1,1),$$

$$\sigma^* = \sqrt{\tau_1^{-1}\kappa(1,1)}, \quad \zeta(t) = \tau_t \int_0^t \tau_s^{-1}\alpha_s ds, \quad \rho_t = \frac{\int_0^t \tau_s^{-2} g_s^2 ds}{\int_0^1 \tau_s^{-2} g_s^2 ds}.$$

Now we prove Theorem 3.2.

Proof of Theorem 3.2. We shall apply Theorem D.3 to the Gaussian SB (14) by setting $\mu_0 := Z_0$, $\mu_1 = Z_1$, $\Sigma_0 = \Sigma_1 := \sigma_{min}^2 I$, $\alpha_t := \dot{a}_t Z_0 + \dot{b}_t Z_1$, $c_t := 0$, and $g_t := \omega$. Then, we have $\tau_t = 1$, $\kappa(t,t') = \omega^2 t$, $r_t = t$, $\sigma^* = \omega$, $\zeta(t) = \int_0^t \alpha_s ds = \left(\int_0^t \dot{a}_s ds\right) Z_0 + \left(\int_0^t \dot{b}_s ds\right) Z_1 = (a_t - a_0)Z_0 + (b_t - b_0)Z_1$, and $\rho_t = t$. Also, $D_{\sigma^*} = (4\sigma_{min}^4 + \omega^4)^{1/2} I$ and $C_{\sigma^*} = C_{\sigma^*}^T = \frac{1}{2}((4\sigma_{min}^4 + \omega^4)^{1/2} - \omega^2)I$.

Thus,

$$\mu_t = (1-t)Z_0 + tZ_1 + (a_t - a_0)Z_0 + (b_t - b_0)Z_1 - t[(a_1 - a_0)Z_0 + (b_1 - b_0)Z_1] \tag{65}$$

and

$$\Sigma_t = [((1-t)^2 + t^2)\sigma_{min}^2 + t(1-t)((4\sigma_{min}^4 + \omega^4)^{1/2} - \omega^2) + \omega^2 t(1-t)]I \tag{66}$$

$$= \sigma_{min}^2 + \left(\sqrt{4\sigma_{min}^4 + \omega^4} - 2\sigma_{min}^2\right) \cdot t(1-t). \tag{67}$$

Theorem 3.2 then follows from Theorem D.3 with the above formula for μ_t and Σ_t. □

D.4 Comparing the Variance of Different Vector Field Models

We begin with providing intuitions for understanding our proposed probability path model. We expect that our model improves upon the other considered models, as it takes advantage of the inherent continuity and correlation in the spatio-temporal data. Intuitively, for time series samples whose underlying dynamics are continuous and obey a physical law, a Gaussian sample is typically further from the time series samples, so the distance between a Gaussian sample and a time series sample should generally be larger than the distance between consecutive time series samples (which can be highly correlated). Therefore, using a probability path that connects consecutive time series samples could lead to faster convergence and more stable training, when compared to using a path that simply connects a time series sample to a Gaussian sample, since the resulting flow model in the former case can better capture the true system dynamics with less effort.

Moreover, if the consecutive samples are sufficiently correlated, then the variance of the VF corresponding to our proposed probability path model can be lower than the variance of the VF corresponding to the other choices of probability paths. Precise statements capturing this are the contents of Theorem 3.3, which focuses on comparison between our proposed model and the optimal transport VF model of (Lipman et al., 2022).

Before proving Theorem 3.3, we start with the following lemma.

Lemma D.4. *Let A, B, C, D be random vectors where C and D are independent, both A and B are independent of C and D (but A and B could be dependent). If $Cov(A,B) \geq (Var(C) - Var(D) + Var(B))/2$, then*

$$Var(A+D) \geq Var(A-B+C) = Var(B-A+C), \tag{68}$$

where $A \geq B$ means that $A - B$ is positive semidefinite.

Proof. We compute:

$$\begin{aligned}
Var(A+D) &= Var(A-B+C+B+D-C) && (69)\\
&= Var(A-B+C) + Var(B+D) + Var(C) + 2Cov(A-B+C, B+D)\\
&\quad - 2Cov(A-B+C, C) - 2Cov(B+D, C) && (70)\\
&= Var(A-B+C) + Var(B+D) - Var(C) + 2Cov(A-B+C, B)\\
&\quad + 2Cov(A-B+C, D) && (71)\\
&= Var(A-B+C) + Var(B+D) - Var(C) + 2Cov(A,B) - 2Var(B) && (72)\\
&= Var(A-B+C) - Var(C) + Var(D) + 2Cov(A,B) - Var(B), && (73)
\end{aligned}$$

where we have simply rearranged the terms in the first equality, used the formula $Var(A+B+C) = Var(A) + Var(B) + Var(C) + 2Cov(A,B) + 2Cov(A,C) + 2Cov(B,C)$, bilinearity of covariance, the facts that $Cov(A,A) = Var(A)$ and $Var(cA) = c^2 A$ for a scalar c, as well as the assumption that both A and B are independent of C, D in the last four equalities.

Therefore, if $-Var(C)+Var(D)+2Cov(A,B)-Var(B)\geq 0$, then we have $Var(A+D)\geq Var(A-B+C)$. □

Now we prove Theorem 3.3.

Proof. Note that $c_t' = \frac{\sigma^2(1-2t)}{2\sqrt{\sigma_{min}^2+\sigma^2 t(1-t)}}$, $Var(c_t'\xi) = (c_t')^2 I$ and $Var(-\eta) = I$. Therefore, using these and applying Lemma D.4 with $A := z^{\tau-1}$, $B := z^{\tau}$, $C := c_t'\xi$ and $D := -\eta$, allow us to establish the claim that $Var(\tilde{u}_t(Z_t|z^{\tau-1})) \geq Var(u_t(Z_t|z^{\tau-1}, z^{\tau}))$ if

$$Cov(z^{\tau-1}, z^{\tau}) \geq \frac{1}{2}\left(\frac{\sigma^4(1-2t)^2 I}{4(\sigma_{min}^2+\sigma^2 t(1-t))} + Var(z^{\tau}) - I\right). \tag{74}$$

Since the function $f(t) := \frac{\sigma^4(1-2t)^2}{4(\sigma_{min}^2+\sigma^2 t(1-t))}$ is maximized at the endpoints $t = 0, 1$ with the maximum value of $\sigma^4/4\sigma_{min}^2$, the desired result stated in the theorem follows. □

Lastly, we provide some discussions following Theorem 3.3 (using the notations there).

Discussions. Let us denote $v_t^\theta(Z) := v_t^\theta(z^\tau, z^{\tau-1}, \xi)$ to show the explicit dependence of the vector field neural net on the random samples t, z^τ, $z^{\tau-1}$ and $\xi \sim \mathcal{N}(0, I)$ drawn during each update of gradient descent during training. During each gradient descent update, our model involves computation of

$$\nabla_\theta \mathcal{L}_{cfm}(\theta; t, \xi, z^\tau, z^{\tau-1}) = 2\nabla_\theta v_t^\theta(z^\tau, z^{\tau-1}, \xi)^T \cdot (v_t^\theta(z^\tau, z^{\tau-1}, \xi) - u_t(Z_t|z^\tau, z^{\tau-1})) \tag{75}$$

$$=: 2\nabla_\theta v_t^\theta(z^\tau, z^{\tau-1}, \xi)^T \cdot \Delta_t^\theta(z^{\tau-1}, z^\tau, \xi), \tag{76}$$

with $t \sim \mathcal{U}[0,1]$, $\xi \sim \mathcal{N}(0, I)$ and the latent samples $z^\tau, z^{\tau-1}$ drawn randomly.

Similarly, for the rectified flow model let us denote $\tilde{v}_t^\theta(Z) := v_t^\theta(z^{\tau-1}, \eta)$ to show the explicit dependence of the vector field neural net on the random samples t, $z^{\tau-1}$ and $\eta \sim \mathcal{N}(0, I)$ drawn during each update of gradient descent during training. Each update of gradient descent using the rectified flow model involves computation of

$$\nabla_\theta \tilde{\mathcal{L}}_{cfm}(\theta; t, \eta, z^{\tau-1}) = 2\nabla_\theta \tilde{v}_t^\theta(z^{\tau-1}, \eta)^T \cdot (\tilde{v}_t^\theta(z^{\tau-1}, \eta) - \tilde{u}_t(\tilde{Z}_t|z^{\tau-1})) \tag{77}$$

$$=: 2\nabla_\theta \tilde{v}_t^\theta(z^{\tau-1}, \eta)^T \cdot \tilde{\Delta}_t^\theta(z^{\tau-1}, \eta), \tag{78}$$

with $t \sim \mathcal{U}[0,1]$, $\eta \sim \mathcal{N}(0, I)$ and the latent sample $z^{\tau-1}$ drawn randomly.

Lower gradient variance results in smoother training loss curve and potentially faster convergence, so it is useful to compare the variances of the loss gradient for the two models. However, the variances are highly dependent on $\nabla_\theta v_t^\theta$, $\nabla_\theta \tilde{v}_t^\theta$ and their covariance with the other random vectors appearing in Eq. (75) and Eq. (77), making such comparison challenging without strong assumptions. Heuristically, the difference in the variances of the loss gradient during each update for the two models is primarily determined by the difference between $Var(\Delta_t^\theta(z^{\tau-1}, z^\tau, \xi))$ and $Var(\tilde{\Delta}_t^\theta(z^{\tau-1}, \eta))$ if $\nabla_\theta v_t^\theta$ and $\nabla_\theta \tilde{v}_t^\theta$ are relatively stable. In this case, we have $Var(\Delta_t^\theta(z^{\tau-1}, z^\tau, \xi)) \leq Var(\tilde{\Delta}_t^\theta(z^{\tau-1}, \eta))$ if we suppose the assumptions in Theorem 3.3, $Var(\tilde{v}_t^\theta) \geq Var(v_t^\theta)$ and $Cov(v_t^\theta, u_t) \geq Cov(\tilde{v}_t^\theta, \tilde{u}_t)$.

The implications of Theorem 3.3 together with the heuristics above could partially explain why our probability path model leads to smoother loss curve and faster convergence (see Figure 3) compared to the RIVER method of (Davtyan et al., 2023). On the other hand, the dependence of the lower bound in the theorem on σ and σ_{min} suggests that using values of σ that is relatively large enough might not keep the variance of the vector field low, which could partially explain the phenomenon displayed in Figure 3, where using $\sigma = 0.1$ and $\sigma_{min} = 0.001$ leads to large loss fluctuations.

E Additional Empirical Results

In this section, we provide additional experimental results.

E.1 Visualization of Flow Patterns and Dynamics

Figure 2 provides visual results of the predicted snapshots by our model for each task. The visualizations highlight our model's ability to capture complex flow patterns and dynamics.

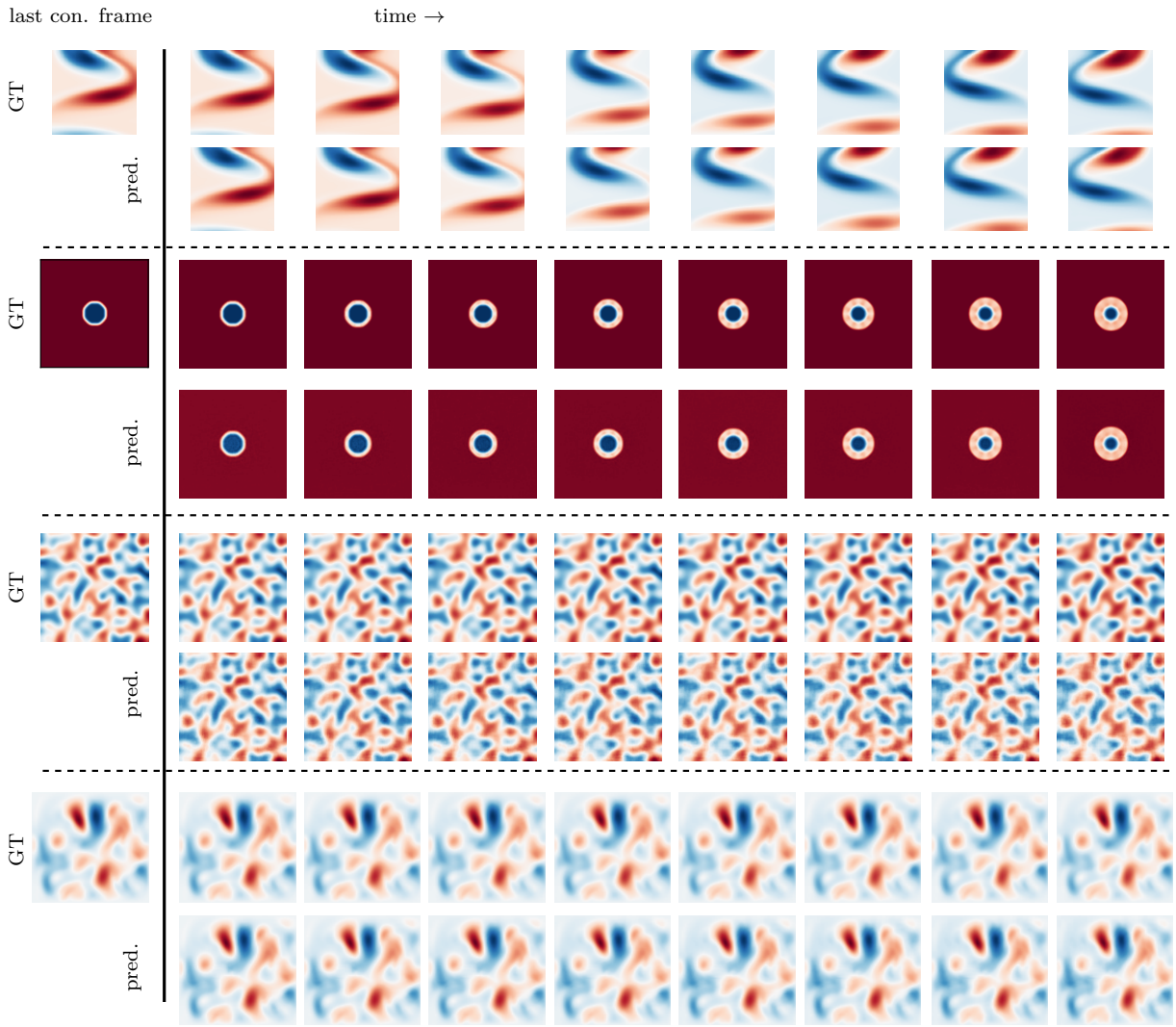

Figure 2: Visualization of predicted frames using our model of probability path for the considered tasks. From top to bottom: fluid flow past a cylinder, shallow-water equation, diffusion-reaction equation, and incompressible Navier-Stokes equation. In each case, GT indicates the ground truth frames and pred. indicates the predicted frames.

E.2 Ablation Studies

To further assess our model, we conducted an ablation study focusing on the impact of various hyperparameters. Specifically, we study the impact of the values of σ, the choice of sampler, and the number of sampling steps during inference. For small σ_{sam}, we find that this parameter has negligible impact on test performance, so we fixed $\sigma_{\text{sam}} = 0$ for all experiments in this section.

Impact of σ on training stability. Figure 4 illustrates the effect of different σ values on the training loss curve for our method on the fluid flow past a cylinder task. We observed that larger values of σ (e.g., $\sigma = 0.1$) resulted in smoother loss curves and more stable convergence during training.

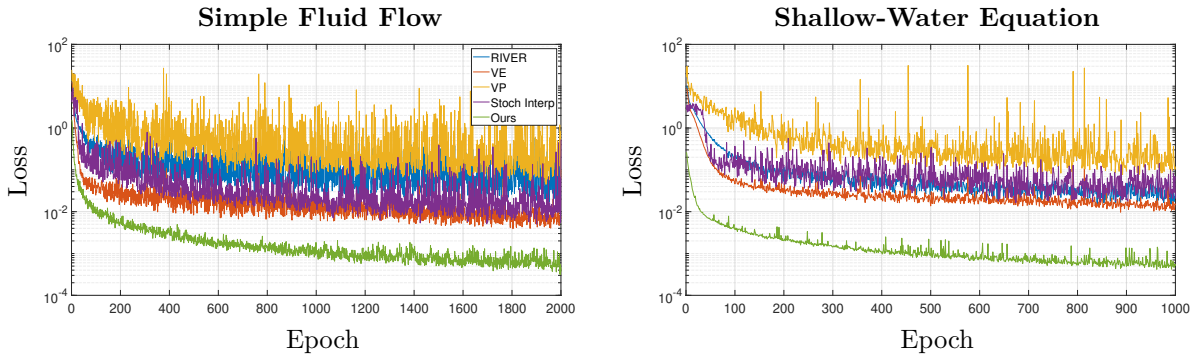

Figure 3: Training loss for different models of probability path for the fluid flow past a cylinder task. Our model leads to fastest convergence and smoothest loss curve among all models.

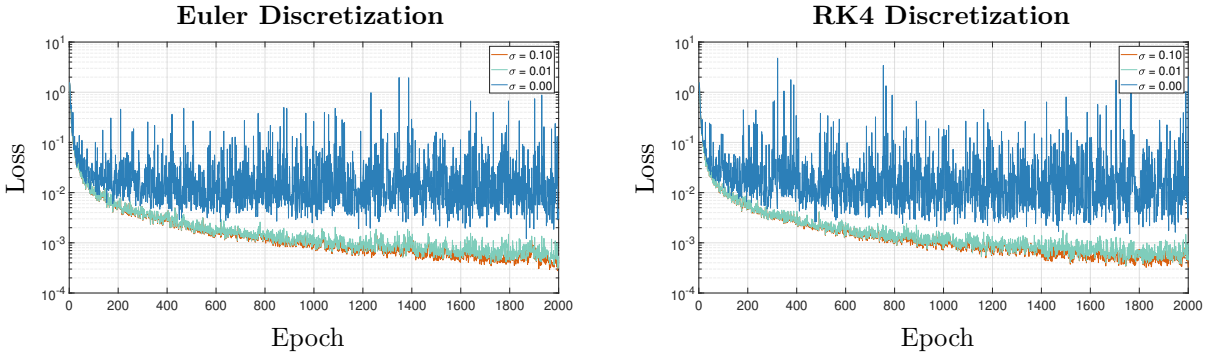

Figure 4: Training loss for different values of σ using our probability path model. The left subplot shows results for the Euler sampler, and the right subplot for the RK4 sampler. We see that the loss curve is sensitive to the choice of σ, with larger values of σ giving smoother loss curves.

Effect of σ, sampler choice, and sampling steps on test performance. Table 3 investigates how different values of σ, the choice of sampler (Euler or RK4), and the number of sampling steps affect test performance. It can be seen, that even with as few as 5 sampling steps using the Euler scheme, our model perform reasonably well. However, increasing the number of sampling steps or employing the more computationally intensive RK4 sampler can help to lead to better results.

F Experimental Details

In this section, we provide the experimental details for the tasks considered in Section 5.

F.1 Details on the Datasets

Fluid flow past a cylinder (FPC). We use the fluid flow past a stationary cylinder at a Reynolds number of 100 as a simple test problem. This fluid flow is a canonical problem in fluid dynamics characterized by a periodically shedding wake structure (Erichson et al., 2020; 2019). The flow dynamics are governed by the two-dimensional incompressible Navier–Stokes equations:

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \mathbf{u},$$

$$\nabla \cdot \mathbf{u} = 0,$$

Table 3: Ablation study for the fluid flow past a cylinder task. Results are averaged over 5 generations.

σ	sampler	sampling steps	Test MSE (↓)	Test RFNE (↓)	PSNR (↑)	SSIM (↑)
0.0	Euler	5	1.78e-03	4.50e-02	44.12	0.98
0.01	Euler	5	1.79e-03	4.50e-02	44.13	0.98
0.1	Euler	5	1.94e-03	4.50e-02	44.26	0.98
0.0	Euler	10	7.14e-04	2.90e-02	47.07	0.99
0.01	Euler	10	3.81e-04	2.30e-02	48.73	0.99
0.1	Euler	10	2.83e-03	5.10e-02	44.14	0.98
0.0	RK4	10	3.89e-04	2.20e-02	49.22	0.99
0.01	RK4	10	3.80e-04	2.30e-02	48.89	0.99
0.1	RK4	10	6.49e-03	7.80e-02	40.70	0.97
0.0	Euler	20	5.51e-04	2.70e-02	47.44	0.99
0.01	Euler	20	7.32e-04	3.10e-02	46.85	0.99
0.1	Euler	20	7.93e-04	3.10e-02	46.80	0.99
0.0	RK4	20	9.31e-04	3.30e-02	46.42	0.99
0.01	RK4	20	6.62e-04	2.80e-02	47.62	0.99
0.1	RK4	20	6.58e-04	2.90e-02	47.14	0.99

where $\mathbf{u} = (u, v)$ is the velocity field, p is the pressure, ρ is the fluid density, and ν is the kinematic viscosity. The vorticity field ω is obtained from the velocity field via:

$$\omega = \nabla \times \mathbf{u},$$

providing insights into the rotational characteristics of the flow.

For simulating the data, the Immersed Boundary Projection Method (IBPM) has been used (Colonius & Taira, 2008). The flow tensor has dimensions $199 \times 449 \times 151$, representing 151 temporal snapshots on a 449×199 spatial grid. We crop and spatially subsample the data which results in a 64×64 spatial field.

Shallow-water equation (SWE). The shallow-water equations, derived from the compressible Navier-Stokes equations, can be used for modeling free-surface flow problems. We consider the 2D equation used in (Takamoto et al., 2022), which is the following system of hyperbolic PDEs:

$$\partial_t h + \nabla h\mathbf{u} = 0, \quad \partial_t h\mathbf{u} + \nabla\left(\mathbf{u}^2 h + \frac{1}{2} g_r h^2\right) = -g_r h \nabla b, \tag{79}$$

where $\mathbf{u} = u, v$ being the velocities in the horizontal and vertical direction respectively, h describes the water depth, and b describes a spatially varying bathymetry. $h\mathbf{u}$ can be interpreted as the directional momentum components and g_r describes the gravitational acceleration. The mass and momentum conservation properties can hold across shocks in the solution and thus challenging datasets can be generated. This equation finds application in modeling tsunamis and flooding events.

We use the dataset generated and provided by PDEBench (Takamoto et al., 2022). The data file (`2D_rdb_NA_NA.h5`) can be downloaded from `https://github.com/pdebench/PDEBench/tree/main/pdebench/data_download`. The data sample is a series of 101 frames at a 128×128 pixel resolution and come with 1 channel. The simulation considered in (Takamoto et al., 2022) is a 2D radial dam break scenario. On a square domain $\Omega = [-2.5, 2.5]^2$, the water height is initialized as a circular bump in the center of the domain:

$$h(t = 0, x, y) = \begin{cases} 2, & \text{for } r < \sqrt{x^2 + y^2}, \\ 1, & \text{for } r \geq \sqrt{x^2 + y^2}, \end{cases}$$

with the radius r randomly sampled from $\mathcal{U}(0.3, 0.7)$. The dataset is simulated with a finite volume solver using the *PyClaw* package. We apply standardization and then normalization to the range of $[-1, 1]$ to preprocess the simulated data.

Incompressible Navier-Stokes equation (NSE). The Navier-Stokes equation is the incompressible version of the compressible Navier-Stokes equation, and it can be used to model hydromechanical systems, turbulent dynamics and weather. We use the inhomogeenous version of the equation (which includes a vector field forcing term $\mathbf{u}$) considered by (Takamoto et al., 2022):

$$\nabla \cdot \mathbf{v} = 0, \quad \rho(\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v}) = -\nabla p + \eta \Delta \mathbf{v} + \mathbf{u}, \tag{80}$$

where ρ is the mass density, $\mathbf{v}$ is the fluid velocity, p is the gas pressure and η is shear viscosity. The initial conditions $\mathbf{v}_0$ and inhomogeneous forcing parameters $\mathbf{u}$ are each drawn from isotropic Gaussian random fields with truncated power-law decay τ of the power spectral density and scale σ, where $\tau_{v_0} = -3$, $\sigma_{v_0} = 0.15$, $\tau_u = -1$, $\sigma_u = 0.4$. The domain is taken to be the unit square $\Omega = [0, 1]^2$ and the viscosity $\eta = 0.01$. The equation is numerically simulated using *Phiflow*. Boundary conditions are taken to be Dirichlet to clamp the field velocity to zero at the perimeter.

We use the dataset generated and provided by PDEBench (Takamoto et al., 2022). The data file (`ns_incom_inhom_2d_512-0.h5`) can be downloaded from `https://github.com/pdebench/PDEBench/tree/main/pdebench/data_download`. The data sample is a series of 1000 frames at a 512×512 pixel resolution and come with 2 channels. We do not apply any data preprocessing procedure here.

Diffusion-reaction equation (DRE). We use the 2D extension of diffusion-reaction equation of (Takamoto et al., 2022) which describes two non-linearly coupled variables, namely the activator $u = u(t, x, y)$ and the inhibitor $v = v(t, x, y)$. The equation is given by:

$$\partial_t u = D_u \partial_{xx} u + Du \partial_{yy} u + R_u, \tag{81}$$

$$\partial_t v = D_v \partial_{xx} v + D_v \partial_{yy} v + R_v, \tag{82}$$

where D_u and D_v are the diffusion coefficient for the activator and inhibitor respectively, $R_u = R_u(u, v)$ and $R_v = R_v(u, v)$ are the activator and inhibitor reaction function respectively. The domain of the simulation includes $x \in (-1, 1)$, $y \in (-1, 1)$, $t \in (0, 5]$. This equation can be used for modeling biological pattern formation.

The reaction functions for the activator and inhibitor are defined by the Fitzhugh-Nagumo equation as: $R_u(u, v) = u - u^3 - k - v$, $R_v(u, v) = u - v$, where $k = 5 \times 10^{-3}$, and the diffusion coefficients for the activator and inhibitor are $D_u = 1 \times 10^{-3}$ and $D_v = 5 \times 10^{-3}$ respectively. The initial condition is generated as standard Gaussian noise $u(0, x, y) \sim \mathcal{N}(0, 1.0)$ for $x \in (-1, 1)$ and $y \in (-1, 1)$. We take a no-flow Neumann boundary condition: $D_u \partial_x u = 0$, $D_v \partial_x v = 0$, $D_u \partial_y u = 0$, and $D_v \partial_y v = 0$ for $x, y \in (-1, 1)^2$.

We use a downsampled version of the dataset provided by PDEBench (Takamoto et al., 2022). The data file (`2D_diff-react_NA_NA.h5`) can be downloaded from `https://github.com/pdebench/PDEBench/tree/main/pdebench/data_download`. The data sample is a series of 101 frames at a 128×128 pixel resolution and come with 2 channels. The sample frames are generated using the finite volume method for spatial discretization, and the time integration is performed using the built-in fourth order Runge-Kutta method in the *scipy* package. We do not apply any data preprocessing procedure here.

F.2 Details on Pre-Training the Autoencoder

We provide details on pre-training the autoencoder here. The choice of first pre-training an autoencoder is motivated by the computational challenges of working directly with the high-dimensional spatial resolution of PDE datasets. Training directly in the ambient space requires substantial GPU memory and computational resources, making it impractical for large-scale or high-resolution datasets. By leveraging a latent-space representation, we achieve significant dimensionality reduction while preserving the essential structure of the data, enabling efficient training and inference with standard hardware configurations. For these datasets, latent-space modeling provides a critical balance between computational efficiency, scalability, and performance.

We use the same architecture for the encoder and decoder for all the tasks, with the architecture parameters chosen based on the complexity of the task.

The encoder. The encoder first applies a 2D convolution (`conv_in`) to the input frame, which reduces the number of channels from `in_channels` to `mid_channels`, and processes the spatial dimensions. Then, a series of ResidualBlock layers, which progressively process and downsample the feature map, making it smaller in spatial dimensions but more enriched in terms of features, are applied. After the residual blocks, the feature map undergoes an attention process via a multi-head attention layer. This layer helps the encoder focus on important parts of the input, learning relationships between spatial positions in the image. For the post-attention step, the feature map is further processed by residual blocks and normalized, preparing it for the final convolution. The output of the encoder is obtained by applying a final 2D convolution (`out_conv`), which maps the processed feature map to the desired number of output channels (`out_channels`).

The decoder. The decoder takes the encoded feature map and transforms it back into an output with similar spatial dimensions as the input. Similar to the encoder, the decoder starts with a convolution that adjusts the number of channels from `in_channels` to `mid_channels`. Then, an attention mechanism (similar to the encoder) is applied to focus on important aspects of the encoded features. Next, a series of ResidualBlock layers, combined with UpBlock layers, are used to progressively increase the spatial dimensions of the feature map (upsampling), undoing the compression applied by the encoder. After the upsampling, the output is normalized and passed through a final convolution (`out_conv`), mapping the internal feature representation to the desired number of output channels (`out_channels`).

Table 4 summarizes the architecture parameters used for the considered tasks.

Table 4: Parameters chosen for the encoder (decoder) architecture.

Task	Fluid flow	Shallow-water eq.	Navier-Stokes eq.	Diffusion-reaction eq.
`in_channels`	1 (1)	1 (1)	2 (2)	2 (2)
`out_channels`	1 (1)	1 (1)	2 (2)	2 (2)
`mid_channels`	64 (128)	128 (256)	128 (256)	128 (256)

Training details. We train the autoencoder using AdamW with batch size of 32, no weight decay and $\beta = (0.9, 0.999)$. We use the cosine learning rate scheduler with warmup. For the fluid flow past a cylinder task, we train for 2000 epochs and use learning rate of 0.001. For the Navier-Stokes task, we train for 500 epochs and use learning rate of 0.0001. For the other two tasks we train for 5000 epochs and use learning rate of 0.0005. Our implementation is in PyTorch, and all experiments are run on an NVIDIA A100-SXM4 GPU with 40 GB VRAM belonging to an internal SLURM cluster.

F.3 Details on Training the Flow Matching Models

Architecture. The vector field regressor is a transformer-based model designed to process latent vector fields and predict refined outputs with spatial and temporal dependencies. It uses key parameters like `depth` and `mid_depth`, which control the number of transformer encoder layers in the input, middle, and output stages. The `state_size` and `state_res` parameters define the number of channels and spatial resolution of the input data, while `inner_dim` sets the embedding dimension for processing. The model uses learned positional encodings and a time projection to incorporate spatial and temporal context into the input, which can include `input_latents`, `reference_latents`, and `conditioning_latents`. The input is projected into the inner dimension and passed through a series of transformer layers, with intermediate outputs from the input blocks concatenated with the output layers to refine predictions. Finally, the model projects the processed data back to the original spatial resolution and channel size using BatchNorm, producing the final vector field output.

Table 5 summarizes the architecture parameters used for the considered tasks.

Training details. For all the considered tasks, we train the regressor using AdamW with batch size of 32, learning rate of 0.0005, no weight decay and $\beta = (0.9, 0.999)$. We use the cosine learning rate scheduler with warmup. For the fluid flow past cylinder, we train for 2000 epochs, for the shallow-water equation and diffusion-reaction task we train for 1000 epochs, and for the Navier-Stokes task we train for 100 epochs. Our

Table 5: Parameters chosen for the vector field neural network.

Parameter	Fluid flow	Shallow-water eq.	Navier-Stokes eq.	Diffusion-reaction eq.
`state_size`	4	4	8	4
`state_res`	[8,8]	[16, 16]	[64, 64]	[16, 16]
`inner_dim`	512	512	512	512
`depth`	4	4	4	4
`mid_depth`	5	5	5	5

implementation is in PyTorch, and all experiments are run on an NVIDIA A100-SXM4 GPU with 40 GB VRAM belonging to an internal SLURM cluster.

F.4 Details on the Evaluation Metrics

In addition to the standard mean squared error and relative Frobenius norm error (RFNE), we use the Pearson correlation coefficient to measure the linear relationship between the forecasted frames and the target frames. The range of this coefficient is $[-1, 1]$, with zero implying no correlation. Correlations of -1 or $+1$ imply an exact linear relationship. Positive correlations imply that as x increases, so does y. Negative correlations imply that as x increases, y decreases. In addition, we use peak signal-to-noise ratio (PSNR) to evaluate the quality of signal representation against corrupting noise, and structural similarity index measure (SSIM) (Wang et al., 2004) to assess perceptual results. The presented results are computed by averaging over batch size and number of sample generations.

F.5 Standard Deviations for the Presented Results

Table 6-10 provide the standard deviation of the results presented in the main paper.

Table 6: Standard deviation results for the fluid flow past a cylinder task using different choices of probability paths for flow matching. Results are averaged over 5 generations.

Model	Test MSE (↓)	Test RFNE (↓)	PSNR (↑)	SSIM (↑)
RIVER	1.33e-03	3.09e-02	1.31	5.93e-03
VE-diffusion	1.75e-02	3.60e-01	3.25e-01	2.31e-02
VP-diffusion	1.75e-02	3.60e-01	3.25e-01	2.31e-02
Stochastic interpolant	5.45e-05	3.51e-02	7.74e-02	3.75e-04
Ours ($\sigma = 0.01$, $\sigma_{sam} = 0$, Euler)	6.66e-06	4.49e-03	5.34e-02	3.48e-05

Table 7: Standard deviation for the results of ablation study for the fluid flow past a cylinder task. Results are averaged over 5 generations.

σ	sampler	sampling steps	Test MSE (↓)	Test RFNE (↓)	PSNR (↑)	SSIM (↑)
0.0	Euler	5	3.57e-05	2.42e-02	3.98e-02	2.51e-04
0.01	Euler	5	2.89e-05	2.45e-02	3.01e-02	1.80e-04
0.1	Euler	5	1.64e-05	2.73e-02	2.11e-02	7.21e-05
0.0	Euler	10	9.08e-06	1.25e-02	4.08e-02	5.73e-05
0.01	Euler	10	6.66e-06	4.49e-03	5.34e-02	3.48e-05
0.1	Euler	10	2.84e-05	4.00e-02	3.76e-02	2.21e-04
0.0	RK4	10	3.36e-06	7.69e-03	3.08e-02	2.33e-05
0.01	RK4	10	3.14e-06	5.43e-03	2.56e-02	2.22e-05
0.1	RK4	10	5.88e-05	5.83e-02	2.03e-2	1.85e-04
0.0	Euler	20	6.35e-06	7.36e-03	3.90e-02	5.90e-05
0.01	Euler	20	9.64e-06	1.21e-02	4.30e-02	5.94e-05
0.1	Euler	20	5.44e-06	1.39e-02	1.39e-02	1.03e-04
0.0	RK4	20	1.09e-05	1.65e-02	3.23e-02	8.08e-05
0.01	RK4	20	8.35e-06	1.32e-02	3.29e-02	6.54e-05
0.1	RK4	20	3.44e-06	1.07e-02	1.08e-02	4.08e-05

Table 8: Standard deviation results for the shallow-water equation task using different choices of probability paths for flow matching. Results are averaged over 5 generations.

Model	Test MSE (↓)	Test RFNE (↓)	PSNR (↑)	SSIM (↑)
RIVER	2.81e-05	8.72e-02	1.01e-01	1.29e-03
VE-diffusion	5.01e-04	3.16e-01	3.50e-01	3.25e-03
VP-diffusion	1.56e-04	1.36e-02	2.61e-01	1.06e-01
Stochastic interpolant	7.25e-06	1.03e-01	3.45e-02	4.61e-04
Ours ($\sigma = 0.01$, $\sigma_{sam} = 0$, RK4)	1.54e-06	7.30e-02	3.54e-03	2.60e-04

Table 9: Standard deviation results for the diffusion-reaction equation task using different choices of probability paths for flow matching. Results are averaged over 5 generations.

Model	Test MSE (↓)	Test RFNE (↓)	PSNR (↑)	SSIM (↑)
RIVER	4.93e-04	2.27e-01	7.01e-01	1.82e-02
VE-diffusion	6.65e-03	1.04	5.59e-01	9.11e-03
VP-diffusion	6.75e-04	5.67e-01	1.62	2.13e-02
Stochastic interpolant	7.92e-04	1.14	9.58e-02	1.20e-03
Ours ($\sigma = 0$, $\sigma_{sam} = 0$, RK4)	1.02e-06	4.76e-02	7.96e-03	1.11e-04

Table 10: Standard deviation results for the Navier-Stokes equation task using different choices of probability paths for flow matching. Results are averaged over 5 generations.

Model	Test MSE (↓)	Test RFNE (↓)	PSNR (↑)	SSIM (↑)
RIVER	5.79e-05	2.46e-01	6.14e-01	1.13e-02
VE-diffusion	1.21e-04	1.36	8.82e-02	1.12e-03
VP-diffusion	2.55e-06	1.42e-01	8.28e-02	6.43e-04
Stochastic interpolant	2.03e-07	1.29e-01	9.54e-03	1.95e-04
Ours ($\sigma = 0.01$, $\sigma_{sam} = 0$, RK4)	5.76e-08	4.88e-02	9.32e-03	7.42e-05