SiT: Exploring Flow and Diffusion-based Generative Models with Scalable Interpolant Transformers

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Abstract. We present Scalable Interpolant Transformers (SiT), a family of generative models built on the backbone of Diffusion Transformers (DiT). The interpolant framework, which allows for connecting two distributions in a more flexible way than standard diffusion models, makes possible a modular study of various design choices impacting generative models built on dynamical transport: learning in discrete or continuous time, the objective function, the interpolant that connects the distributions, and deterministic or stochastic sampling. By carefully introducing the above ingredients, SiT surpasses DiT uniformly across model sizes on the conditional ImageNet 256×256 and 512×512 benchmark using the exact same model structure, number of parameters, and GFLOPs. By exploring various diffusion coefficients, which can be tuned separately from learning, SiT achieves an FID-50K score of 2.06 and 2.62, respectively. Code is available here: https://github.com/willisma/SiT

1 Introduction

Contemporary success in image generation has come from a combination of algorithmic advances, improvements in model architecture, and progress in scaling neural network models and data. State-of-the-art diffusion models [24, 48] proceed by incrementally transforming data into Gaussian noise as prescribed by an iterative stochastic process, which can be specified either in discrete or continuous time. At an abstract level, this corruption process can be viewed as defining a time-dependent distribution that is iteratively smoothed from the original data distribution into a standard normal distribution. Diffusion models learn to reverse this corruption process and push Gaussian noise backwards along this connection to obtain data samples. The objects learned to perform this transformation conventionally predict either the noise in the corruption process [24] or the score of the distribution that connects the data and the Gaussian [59], though alternatives of these choices exist [27, 51]. While diffusion models originally represented these objects with a U-Net architecture [24, 49], recent work has highlighted that architectural advances in vision such as the

[†] Equal advising.

Table 1: Scalable Interpolant Transformers. We systematically vary the following aspects of a generative model: time discretization, model prediction, interpolant, and sampler. The resulting Scalable Interpolant Transformer (SiT) model, under identical training compute, consistently outperforms the Diffusion Transformer (DiT) in generating 256×256 ImageNet images. All models employ a patch size of 2. In this work, we ask the question: What is the source of the performance gain?

Model	Params(M)	Training Step	s FID \downarrow
DiT-S	33	400K	68.4
SiT-S	33	400K	57.6
DiT-B	130	400K	43.5
SiT-B	130	400K	33.0
DiT-L	458	400K	23.3
SiT-L	458	400K	18.8
DiT-XL	675	400K	19.5
SiT-XL	675	400K	17.2
DiT-XL	675	7M	9.6
SiT-XL	675	7M	8.3
DiT-XL (cfg=1.5)	675	7M	2.27
SiT-XL (cfg=1.5)	675	7M	2.06

Vision Transformer (ViT) [20] can be incorporated into the standard diffusion model pipeline to improve performance [45].

Orthogonally, significant research effort has gone into exploring the structure of the noising process, which has been shown to lead to performance benefits [32– 34,55]. Yet, many of these efforts do not move past the notion of passing data through a diffusion process with an equilibrium distribution, which is a restricted type of connection between the data and the Gaussian. Recently-introduced *stochastic interpolants* [2] lift this constraint and introduce more flexibility in the noise-data connection. In this paper, we systematically explore the effect of this flexibility on performance in large scale image generation.

Intuitively, we expect that the difficulty of the *learning problem* can be related to both the specific connection chosen and the object that is learned. Our aim is to clarify these design choices, so as to simplify the learning problem and thereby improve performance. To understand where potential benefits arise in the learning problem, we start with Denoising Diffusion Probabilistic Models (DDPMs) and sweep through adaptations of: (i) which object to learn, and (ii) which interpolant to choose to reveal best practices.

In addition to the learning problem, there is a *sampling problem* that must be solved at inference time. It has been acknowledged for diffusion models that sampling can be either deterministic or stochastic [58], and the choice of sampling method can be made after the learning process. Yet, the diffusion coefficients used for stochastic sampling are typically presented as intrinsically tied to the forward noising process, which need not be the case in general.

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Fig. 1: Selected samples from SiT-XL models trained on ImageNet [50] at 512×512 and 256×256 resolution with cfg = 4.0, respectively.



Fig. 2: SiT improves FID across all model sizes. FID-50K over training iterations for both DiT and SiT. All results are produced by a Euler-Maruyama sampler using 250 integration steps. Across all model sizes, SiT converges much faster.

Throughout this paper, we explore how the design of the interpolant and the use of the resulting model as either a deterministic or a stochastic sampler impact performance. We gradually transition from a typical denoising diffusion model to an interpolant model by taking a series of orthogonal steps in the design space. As we progress, we carefully evaluate how each move away from the diffusion model impacts the performance. In summary, our **main contributions** are:

- We systematically study the SiT design space through the combinations of the four key components: time discretization, model prediction, interpolant, and sampler.
- We provide theoretical motivation for the choice of each component and study how they lead to improved practical performance.
- We exploit the tunability of the diffusion coefficient of the stochastic sampler, and show that its adaptation can tighten control of the KL-divergence between the model and the target. We show how this leads to empirical benefits without any additional re-training.

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- Combining the best design choices identified in each component, our SiT model surpasses Diffusion Transformer(DiT) on both 256×256 and 512×512 image resolution, achieving FID-50K scores of 2.06 and 2.62, respectively, without modifying any structure or hyperparameter of the model.

2 SiT: Scalable Interpolant Transformers

We begin by recalling the main ingredients for building flow-based and diffusionbased generative models.

2.1 Flows and diffusions

Flow and diffusion models both utilize stochastic processes to gradually turn noise $\varepsilon \sim N(0, \mathbf{I})$ into data $\mathbf{x}_* \sim p(\mathbf{x})$ for the generating task. Such time-dependent processes can be summarized as follow

$$\mathbf{x}_t = \alpha_t \mathbf{x}_* + \sigma_t \boldsymbol{\varepsilon},\tag{1}$$

where α_t is a decreasing function of t and σ_t is an increasing function of t. Stochastic interpolants and other flow matching methods [2, 4, 38, 40] restrict the process (1) on $t \in [0, 1]$, and set $\alpha_0 = \sigma_1 = 1$, $\alpha_1 = \sigma_0 = 0$, so that \mathbf{x}_t interpolates exactly between \mathbf{x}_* at time t = 0 and $\boldsymbol{\varepsilon}$ and time t = 1. By contrast, score-based diffusion models [32, 34, 59] set both α_t and σ_t indirectly through a forward-time stochastic differential equation (SDE) with N(0, I) as its equilibrium distribution, i.e. \mathbf{x}_t converges to N(0, I) only if $t \to \infty$.

Despite the nuances in formulating the stochastic processes \mathbf{x}_t , common to both stochastic interpolants and score-based diffusion models is the observation that \mathbf{x}_t can be sampled dynamically using either a reverse-time SDE or a probability flow ordinary differential equation (ODE).

Probability flow ODE. The marginal probability distribution $p_t(\mathbf{x})$ of \mathbf{x}_t in (1) coincides with the distribution of the probability flow ODE with a velocity field

$$\dot{\mathbf{X}}_t = \mathbf{v}(\mathbf{X}_t, t),\tag{2}$$

where $\mathbf{v}(\mathbf{x}, t)$ is given by the conditional expectation

 \mathbf{v}

$$\begin{aligned} \mathbf{(x,t)} &= \mathbb{E}[\dot{\mathbf{x}}_t | \mathbf{x}_t = \mathbf{x}], \\ &= \dot{\alpha}_t \mathbb{E}[\mathbf{x}_* | \mathbf{x}_t = \mathbf{x}] + \dot{\sigma}_t \mathbb{E}[\boldsymbol{\varepsilon} | \mathbf{x}_t = \mathbf{x}]. \end{aligned}$$
(3)

The correspondence between $p_t(\mathbf{x})$ and (2) and the formulation of (3) is derived in Appendix ??. By solving (2) backwards in time from $\mathbf{X}_T = \boldsymbol{\varepsilon} \sim \mathsf{N}(0, \mathbf{I})$, we can generate samples from $p_0(\mathbf{x})$, which approximates the ground-truth data distribution $p(\mathbf{x})$. We refer to (2) as a *flow-based* generative model. *Reverse-time SDE.* The time-dependent probability distribution $p_t(\mathbf{x})$ of \mathbf{x}_t also coincides with the distribution of the reverse-time SDE [5]

$$d\mathbf{X}_t = \mathbf{v}(\mathbf{X}_t, t)dt - \frac{1}{2}w_t \mathbf{s}(\mathbf{X}_t, t)dt + \sqrt{w_t} d\bar{\mathbf{W}}_t,$$
(4)

where $\bar{\mathbf{W}}_t$ is a reverse-time Wiener process, $w_t > 0$ is an arbitrary time-dependent diffusion coefficient, $\mathbf{v}(\mathbf{x}, t)$ is the velocity defined in (3), and $\mathbf{s}(\mathbf{x}, t) = \nabla \log p_t(\mathbf{x})$ is the score. Similar to \mathbf{v} , this score is given by the conditional expectation

$$\mathbf{s}(\mathbf{x},t) = -\sigma_t^{-1} \mathbb{E}[\boldsymbol{\varepsilon} | \mathbf{x}_t = \mathbf{x}].$$
(5)

Again, the correspondence between $p_t(\mathbf{x})$ and (4) and the formulation of (5) is derived in Appendix ??. Solving the reverse SDE (4) backwards in time from $\mathbf{X}_T = \boldsymbol{\varepsilon} \sim \mathsf{N}(0, \mathbf{I})$ enables generating samples from the approximated data distribution $p_0(\mathbf{x}) \sim p(\mathbf{x})$. We refer to (4) as a *stochastic* generative model.

Design choices. Score-based diffusion models typically tie the choice of α_t , σ_t , and w_t in (4) to the drift and diffusion coefficients used in the forward SDE that generates \mathbf{x}_t (see (10) below). The stochastic interpolant framework decouples the formulation of \mathbf{x}_t from the forward SDE and shows that there is more flexibility in the choices of α_t , σ_t , and w_t . Below, we will exploit this flexibility to construct generative models that outperform score-based diffusion models on standard benchmarks in image generation task.

2.2 Estimating the score and the velocity

Practical use of the probability flow ODE (2) and the reverse-time SDE (4) as generative models relies on our ability to estimate the velocity $\mathbf{v}(\mathbf{x}, t)$ and/or score $\mathbf{s}(\mathbf{x}, t)$ fields that enter these equations. The key observation made in score-based diffusion models is that the score can be estimated parametrically as $\mathbf{s}_{\theta}(\mathbf{x}, t)$ using the loss

$$\mathcal{L}_{s}(\theta) = \int_{0}^{T} \mathbb{E}[\|\sigma_{t} \mathbf{s}_{\theta}(\mathbf{x}_{t}, t) + \boldsymbol{\varepsilon}\|^{2}] \mathrm{d}t.$$
(6)

This loss can be derived by using (5) along with standard properties of the conditional expectation. Similarly, the velocity in (3) can be estimated parametrically as $\mathbf{v}_{\theta}(\mathbf{x}, t)$ via the loss

$$\mathcal{L}_{\mathbf{v}}(\theta) = \int_{0}^{T} \mathbb{E}[\|\mathbf{v}_{\theta}(\mathbf{x}_{t}, t) - \dot{\alpha}_{t}\mathbf{x}_{*} - \dot{\sigma}_{t}\boldsymbol{\varepsilon}\|^{2}] \mathrm{d}t.$$
(7)

We note that any time-dependent weight can be included under the integrals in both (6) and (7). These weight factors are key in the context of score-based models when T becomes large [33]; in contrast, with stochastic interpolants where T = 1 without any bias, these weights are less important and might impose numerical stability issue (see Appendix ??).

Model prediction. We observed that only one of $\mathbf{s}_{\theta}(\mathbf{x}, t)$ and $\mathbf{v}_{\theta}(\mathbf{x}, t)$ is needed to be estimated in practice. This follows directly from the constraint

$$\mathbf{x} = \mathbb{E}[\mathbf{x}_t | \mathbf{x}_t = \mathbf{x}], = \alpha_t \mathbb{E}[\mathbf{x}_* | \mathbf{x}_t = \mathbf{x}] + \sigma_t \mathbb{E}[\boldsymbol{\varepsilon} | \mathbf{x}_t = \mathbf{x}],$$
(8)

which can be used to re-express the score (5) in terms of the velocity (3) as

$$\mathbf{s}(\mathbf{x},t) = \sigma_t^{-1} \frac{\alpha_t \mathbf{v}(\mathbf{x},t) - \dot{\alpha}_t \mathbf{x}}{\dot{\alpha}_t \sigma_t - \alpha_t \dot{\sigma}_t}.$$
(9)

We include a detailed derivation in Appendix ??. Notably, given the simply linear relationship posed by (9), we can also express $\mathbf{v}(\mathbf{x}, t)$ in terms of $\mathbf{s}(\mathbf{x}, t)$. We will use this relation to specify our **model prediction**. In our experiments, we typically learn the velocity field $\mathbf{v}(\mathbf{x}, t)$ and use it to express the score $\mathbf{s}(\mathbf{x}, t)$ when using an SDE for sampling.

Note that by our definitions $\dot{\alpha}_t < 0$ and $\dot{\sigma}_t > 0$, so that the denominator of (9) is never zero. Yet, σ_t vanishes at t = 0, making the σ_t^{-1} in (9) cause a singularity¹. This suggests the choice $w_t = \sigma_t$ in (4) to cancel this singularity, for which we will explore the performance in the numerical experiments.

Time discretization. The objective functions specified above are defined over a continuous time domain, as opposed to DDPM which couples the time grid used in learning to that used in sampling. Learning in continuous time allows us to specify a discretization used in sampling *a posteriori*, which allows for flexibility in both sampling efficiency and performance.

2.3 Specifying the interpolating process

In Sec. 2.1 we present the general definition of interpolants (α_t and σ_t) for both stochastic interpolant and score-based diffusion. In this section we dive into more details and specify the three choices of interpolants to explore in the experiments.

Score-based diffusion. We follow [59] and use the standard variance-preserving (VP) SDE in forward-time

$$\mathrm{d}\mathbf{X}_t = -\frac{1}{2}\beta_t \mathbf{X}_t \mathrm{d}t + \sqrt{\beta_t} \mathrm{d}\mathbf{W}_t \tag{10}$$

for some $\beta_t > 0$, \mathbf{x}_t 's perturbation kernel $p_t(\mathbf{x}_t | \mathbf{x}_0) = \mathsf{N}(\alpha_t \mathbf{x}_t, \sigma_t^2 \mathbf{I})$ is defined by

SBDM-VP:
$$\alpha_t = e^{-\frac{1}{2}\int_0^t \beta_s \mathrm{d}s}, \qquad \sigma_t = \sqrt{1 - e^{-\int_0^t \beta_s \mathrm{d}s}}.$$
 (11)

¹ We remark that $\mathbf{s}(\mathbf{x}, t)$ can be shown to be non-singular at t = 0 analytically if the data distribution $p(\mathbf{x})$ has a smooth density [2], though this singularity appears in numerical implementations and losses in general.



Fig. 3: Increasing transformer size increases sample quality. *Best viewed zoomedin.* We sample from all 4 of our SiT model (SiT-S, SiT-B, SiT-L and SiT-XL) after 400K training steps using the same latent noise and class label.

The only design flexibility in (11) comes from the choice of β_t , as it determines both α_t and σ_t^2 . For example, setting $\beta_t = 1$ leads to $\alpha_t = e^{-t}$ and $\sigma_t = \sqrt{1 - e^{-2t}}$. This choice necessitates taking T sufficiently large [24] or searching for more appropriate choices of β_t [16,55,59] to reduce the bias. To be specific, such bias comes from the mismatch between the condition $\varepsilon \sim N(0, \mathbf{I})$ used in practice for sampling and the density of the process $\mathbf{x}_1 \not\sim N(0, \mathbf{I})$, as stated in Sec. 2.1.

General interpolants. In the stochastic interpolant framework, the process (1) is defined explicitly and without any reference to a forward SDE, creating more flexibility in the choice of α_t and σ_t . Specifically, any choice satisfying:

(i) $\alpha_t^2 + \sigma_t^2 > 0$ for all $t \in [0, 1]$; (ii) α_t and σ_t are differentiable for all $t \in [0, 1]$; (iii) $\alpha_1 = \sigma_0 = 0$, $\alpha_0 = \sigma_1 = 1$;

gives a process that interpolates without bias between $\mathbf{x}_{t=0} = \mathbf{x}_*$ and $\mathbf{x}_{t=1} = \boldsymbol{\varepsilon}$. In our numerical experiments, we exploit this design flexibility to test, in particular, the choices

Linear:
$$\alpha_t = 1 - t,$$
 $\sigma_t = t,$
GVP: $\alpha_t = \cos(\frac{1}{2}\pi t),$ $\sigma_t = \sin(\frac{1}{2}\pi t),$ (12)

where GVP refers to a generalized VP which has constant variance across time for any endpoint distributions with the same variance. We note that the fields $\mathbf{v}(\mathbf{x},t)$ and $\mathbf{s}(\mathbf{x},t)$ entering (2) and (4) depend on the choice of α_t and σ_t , and typically must be specified before learning³. This is in contrast to the diffusion coefficient w(t), as we now describe.

² VP is the only linear scalar SDE with an equilibrium distribution [55]; interpolants extend beyond $\alpha_t^2 + \sigma_t^2 = 1$ by foregoing the requirement of an equilibrium distribution.

³ The requirement to learn and sample under one choice of path specified by α_t, σ_t , at training time may be relaxed and is explored in [1].

2.4 Specifying the diffusion coefficient

As stated earlier, the SBDM diffusion coefficient used in (4) is usually taken to match that of (10). That is, one sets $w_t = \beta_t$. In the stochastic interpolant framework, this choice is again subject to greater flexibility: any $w_t \ge 0$ can be used. Interestingly, this choice can be made *after* learning, as it does not affect the velocity $\mathbf{v}(\mathbf{x}, t)$ or the score $\mathbf{s}(\mathbf{x}, t)$. In our experiments, we exploit this flexibility by considering the following choices:

- (i) $w_t = \sigma_t$; this is used to eliminate the singularity at t = 0 following the explanation at the end of Sec. 2.2;
- (ii) $w_t = \sin^2(\pi t)$; this also eliminates the singularity at t = 0, and allows us to explore the effect of removing diffusivity at times close to t = 1 in sampling.
- (iii) w_t can be chosen to minimize an upper bound on the KL divergence $D_{\text{KL}}(p(\mathbf{x})||p_0(\mathbf{x}))$, where $p(\mathbf{x})$ denotes the true data distribution and $p_0(\mathbf{x})$ refers to the density of \mathbf{x}_t at t = 0. Disregarding the simulation cost of integrating the SDE (4), it can be shown (see Appendix ??) that the following choice of w_t minimizes the KL upper bound:

$$w_t = w_t^{\text{KL}} \equiv 2\left(\dot{\sigma}_t \sigma_t - \frac{\dot{\alpha}_t \sigma_t^2}{\alpha_t}\right).$$
(13)

Under the SBDM-VP interpolant, w_t^{KL} coincides with β_t ; this aligns with the claim made in [58].

(iv) If the SDE in (iii) becomes hard to integrate because of the magnitude of w_t^{KL} near t = 1, one may wish to *regularize* the diffusion coefficient to reduce the integration cost. For example, difficulties may arise for the Linear and GVP interpolants, because $w_t^{\text{KL}} \to \infty$ as $t \to 1$ given the presence of α_t in the denominator of (13). Including the integration cost of (4), it can also be shown (see Appendix ??) that an optimal regularized w_t is given by

$$w_t^{\mathrm{KL},\eta} \equiv w_t^{\mathrm{KL}} \sqrt{\frac{\mathcal{L}_t}{\mathcal{L}_t + 2\eta(w_t^{\mathrm{KL}})^2}},\tag{14}$$

where \mathcal{L}_t is the value of \mathcal{L}_v in Sec. 2.2 at time t, and η is any non-negative constant. With $\eta = 0$, we recover w_t^{KL} . For score models, we first convert to a velocity model following (9), then calculate the corresponding \mathcal{L}_v . As $t \to 1$, $w_t^{\text{KL},\eta}$ approaches a limit at $\sqrt{\frac{\mathcal{L}_{t\to 1}}{2\eta}}$. If \mathcal{L}_t is defined everywhere on [0, 1], then $w_t^{\text{KL},\eta}$ will be well-behaved on [0, 1].

2.5 Interpolant Transformer Architecture

The backbone architecture and capacity of generative models are both crucial for producing high-quality samples. In order to eliminate any confounding factors and focus on our exploration, we strictly follow the standard Diffusion Transformer (DiT) [45] and its configurations. This way, we can also test the scalability of our model across various model sizes.

Here we briefly introduce the model design. Generating high-resolution images with diffusion models can be computationally expensive. Latent diffusion models (LDMs) [48] address this by first downsampling images into a smaller latent embedding space using an encoder E, and then training a diffusion model on z = E(x). New images are created by sampling z from the model and decoding it back to images using a decoder x = D(z).

Similarly, SiT is a latent generative model, and we use the same pre-trained VAE encoder and decoder models originally used in Stable Diffusion [48]. SiT processes a spatial input z (shape $32 \times 32 \times 4$ for $256 \times 256 \times 3$ images) by first 'patchifying' it into T linearly embedded tokens of dimension d. We always use a patch size of 2 in these models as they achieve the best sample quality. We then apply standard ViT [20] sinusoidal positional embeddings to these tokens. We use a series of N SiT transformer blocks, each with hidden dimension d.

Our model configurations—SiT-{S,B,L,XL}—vary in model size (parameters) and compute (flops), allowing for a model scaling analysis. For class-conditional generation on ImageNet, we use the AdaLN-Zero block [45] to process additional conditional information (times and class labels). SiT architectural details are listed in Appendix ??.

The complete SiT design space that we explore consists of the choice of time discretization and the model prediction (Sec. 2.2), the choice of the interpolant (Sec. 2.3), the choice of sampler and diffusion coefficient (Sec. 2.4), and the model size (Sec. 2.5).

3 Experiments

To provide a more detailed answer to the question raised in Table 1 and make a fair comparison between DiT and SiT, we gradually transition from a DiT model (discrete, score prediction, VP interpolant) to a SiT model (continuous, velocity prediction, Linear interpolant) and present the impacts on performance.

Experimental setup. In the transition experiments, we use SiT-B models trained on 256×256 image resolution on the ImageNet as our backbone. We fix training steps to be 400K throughout the transition. For solving the ODE (2), we adopt a fixed step second-order Heun integrator; for solving the SDE (4), we used a first-order Euler-Maruyama integrator. With both solver choices we limit the number of function evaluations (NFE) to be 250 to match the number of sampling steps used in DiT. All metrics presented are FID-50K scores evaluated on the ImageNet training set unless otherwise stated.

We also scale up our SiT model to the XL configuration and train on both 256×256 and 512×512 resolution on ImageNet. We strictly follow the training settings of DiT and did not tune any hyperparameters.

3.1 Model Parameterization

Discrete- to continuous-time. Continuous time training has been previously studied from the perspective of improved likelihood bounds [34,59]. As mentioned in Section 2.2, here we focus on the fact that training in continuous time allows us to decouple discretization choices in sampling from the particular training method, which allows for finding the right discretization for various choices of diffusion coefficients that we are free to choose after training. We observe a marginal performance increase in Table 2 by switching to continuous time.

We additionally observe in Figure 5 that flexibility in integration allows one to trade-off number of functional evaluations and FID performance.

Model parameterization. To clarify the role of the model parameterization in the context of SBDM-VP, we now compare learning (i) a score model using (6) (\mathcal{L}_{s}) , (ii) a weighted score model $(\mathcal{L}_{s\lambda})$, or (iii) a velocity model using $(7)(\mathcal{L}_{v})$. We observe a significant performance increase with $\mathcal{L}_{s\lambda}$ and \mathcal{L}_{v} in Table 3.

In accordance with the observation made in [33], we carefully choose a $\lambda(t)$ such that $\lambda_{s_{\lambda}}$ is made equivalent to λ_{v} . We will provide detailed derivations in Appendix ??, and demonstrate such λ is closely related to the maximum likelihood weighting proposed in [58,61]. Furthermore, we note that $\lambda(t) \to \infty$ as $t \to 0$, thus compensating for the vanishing gradient of the score objective when near the data. This could also account for the performance gain from λ_s to $\lambda_{s_{\lambda}}$.

Table 2: Discrete vs. continuous.				Table 3: Effect of parameterization						
	Model	Objectiv	e FID	Interpolant	Model	Objective	FID			
DDPM	Noise	$\mathcal{L}_{ ext{s}}^{N}$	44.2	SBDM-VP	Score	\mathcal{L}_{s}	43.6			
SBDM-VI	P Score	\mathcal{L}_{s}	43.6	SBDM-VP	Score	$\mathcal{L}_{\mathrm{s}_{\lambda}}$	39.1			
				SBDM-VP	Velocity	\mathcal{L}_{v}	39.8			

Choices of interpolant. Sec. 2 highlights that there are many possible ways to build a connection between the data distribution and a Gaussian by varying the choice of α_t and σ_t in the definition of the interpolant (1). To understand the role of this choice, we now study the benefits of moving away from the commonly-used SBDM-VP setup. We consider learning a velocity model $\mathbf{v}(\mathbf{x}, t)$ with the Linear and GVP interpolants presented in (12), which make the interpolation between the Gaussian and the data distribution exact on [0, 1]. We benchmark these models against the SBDM-VP in Table 4, where we find that both the GVP and Linear interpolants obtain significantly improved performance.

One possible explanation for this observation is given in Fig. 4, where we see that the path length (transport cost) is reduced when changing from SBDM-VP to GVP or Linear. We note that this is equivalently reducing curvatures in the ODE trajectories from SBDM-VP to Linear, which is known to reduce the timediscretization errors in sampling [37,40], and thus contributing to the performance. Numerically, we also note that for SBDM-VP, $\dot{\sigma}_t = \beta_t e^{-\int_0^t \beta_s ds}/(2\sigma_t)$ becomes singular at t = 0: this can pose numerical difficulties inside \mathcal{L}_v , leading to difficulty in learning near the data distribution. This issue does not appear with the GVP and Linear interpolants.

Table 4: Effect of interpolant.				_	Table 5:	ODE vs	. SDE, u	$v_t = w$	t^{KL} .
Interpolant	Model	Objective	FID		Interpolant	Model	Objective	ODE	SDE
SBDM-VP	Velocity	\mathcal{L}_{v}	39.8	-	SBDM-VP	Velocity	\mathcal{L}_{v}	39.8	37.8
Linear	Velocity	\mathcal{L}_{v}	34.8		Linear	Velocity	\mathcal{L}_{v}	34.8	33.6
GVP	Velocity	\mathcal{L}_{v}	34.6		GVP	Velocity	\mathcal{L}_{v}	34.6	32.9

3.2 Deterministic vs stochastic sampling

As shown in Sec. 2, given a learned model, we can sample using either the probability flow equation (2) or an SDE (4). In Tab. 5 we illustrate the discrepancy between the two methods when using the same trained velocity model. We find performance improvements by sampling with an SDE over the ODE, which is in line with the bounds given in [2]: the SDE has better control over the KL divergence between the model density at t = 0 and the ground truth data distribution. We also note that the performance of ODE and SDE integrators may differ under different computation budgets. As shown in Fig. 5, the ODE converges faster with fewer NFE, while the SDE is capable of reaching a much lower final FID score when given a larger computational budget.

Tunable diffusion coefficient. Motivated by the improved performance of SDE sampling, we now consider the effect of tuning the diffusion coefficient in inference. As shown in Table 6, we sweep through all different combinations of our model prediction and interpolant, and present the result. We find that the optimal choice for sampling is both *model prediction* and *interpolant* dependent.

According to Sec. 2.4, the choice of $w_t = w_t^{\text{KL}}$ would ideally minimize the upper bound for the KL divergence $D_{\text{KL}}(p(\mathbf{x})|||p_0(\mathbf{x}))$ and make the SDE approximate the data distribution more closely, barring integration costs. This theoretical result is supported by empirical observation for the SBDM-VP and GVP interpolants presented in Table 6. For Linear interpolants, the cost-regularized version $w_t^{\text{KL},\eta}$ provides the best FID, because the SDE for the Linear interpolant with w_t^{KL} becomes hard to integrate at the endpoint. Generally speaking, the score models perform worse than the velocity models, which may be due to the singularity of the objective in (6). Moreover, the efficacy of using w_t^{KL} in this context is also reduced, for similar reason. For example, reverting (9) to obtain $v_{\theta}(\mathbf{x}, t)$





Fig. 4: Path length. The path length $C(v) = \int_0^1 \mathbb{E}[|\mathbf{v}(\mathbf{x}_t, t)|^2] dt$ arising from the velocity field at different training steps; each curve is approximated by 10000 datapoints at each training step.

Fig. 5: Comparison of ODE and SDE \mathbf{w} / choices of diffusion coefficients. We evaluate each sampler using a 400K steps trained SiT-B model with Linear interpolant and learning the $\mathbf{v}(\mathbf{x}, t)$.

Table 6: Evaluation of our SDE samplers. The last three columns specify different diffusion coefficients w_t . To make the SBDM-VP competitive, we perform evaluation on the weighted score model $\mathcal{L}_{s_{\lambda}}$. We mark the optimal w_t for each interpolant.

Interpolant	Model	Objective	$w_t = w_t^{\mathrm{KL}}$	$w_t = \sigma_t$	$w_t = \sin^2(\pi t)$	$w_t = w_t^{\mathrm{KL},\eta}$
SBDM-VP	velocity score	$\mathcal{L}_{\mathrm{v}} \ \mathcal{L}_{\mathrm{s}_{\lambda}}$	37.8 35.7	$38.7 \\ 37.1$	$39.2 \\ 37.7$	$41.1 \\ 38.9$
GVP	velocity score	$\mathcal{L}_{ m v} \ \mathcal{L}_{ m s}$	32.9 37.8	$33.4 \\ 33.5$	$33.6 \\ 33.2$	$33.2 \\ 33.3$
Linear	velocity score	$\mathcal{L}_{\mathrm{v}} \ \mathcal{L}_{\mathrm{s}}$	$\begin{array}{c} 33.6\\ 41.0 \end{array}$	$33.5 \\ 35.3$	$33.3 \\ 34.4$	33.0 34.9

from $s_{\theta}(\mathbf{x}, t)$ will result in a singularity at t = 1 in \mathcal{L}_t used to choose $w_t^{\mathrm{KL},\eta}$ in (14). Lastly, for SBDM-VP we observe worse result from $w_t^{\mathrm{KL},\eta}$ as opposed to w_t^{KL} . Different from Linear and GVP, as stated in Sec. 2.4 and Sec. 3.1, w_t^{KL} is well-defined everywhere on [0, 1] for SBDM-VP, whereas $w_t^{\mathrm{KL},\eta}$ suffers from the singularity issue posed by \mathcal{L}_v near t = 0. These observations supports our claim made before, that the optimal choice of w_t will always be *model prediction* and *interpolant* dependent.

We also note that the influences of different diffusion coefficients can vary across different model sizes. Empirically, we observe the best choice for our SiT-XL is a velocity model with Linear interpolant and sampled with $w_t^{\text{KL},\eta}$.

3.3 Classifier-free guidance

Classifier-free guidance (CFG) [26] often leads to improved performance for score-based models. In this section, we give a concise justification for adopting it on the velocity model, and then empirically show that the drastic gains in performance for DiT case carry across to SiT.

Guidance for a velocity field means that: (i) that the velocity model $\mathbf{v}_{\theta}(\mathbf{x}, t; \mathbf{y})$ takes class labels y during training, where y is occasionally masked with a null token \emptyset ; and (ii) during sampling the velocity used is $\mathbf{v}_{\theta}^{\zeta}(\mathbf{x}, t; \mathbf{y}) = \zeta \mathbf{v}_{\theta}(\mathbf{x}, t; \mathbf{y}) + (1 - \zeta) \mathbf{v}_{\theta}(\mathbf{x}, t; \emptyset)$ for a fixed $\zeta > 0$. In Appendix ??, we show that this indeed corresponds to sampling the tempered density $p(\mathbf{x}_t)p(\mathbf{y}|\mathbf{x}_t)^{\zeta}$ as proposed in [43]. Given this observation, one can leverage the usual argument for classifier-free guidance of score-based models.

We observed similar performance improvement with our SiT-XL models under identical computation budget and CFG scale as DiT-X: models. For SiT-XL 256×256 , we follow identical settings in DiT and train the model for 7M steps. We show samples in Fig. 1, and report the result in Table 7. For SiT-XL 512×512 , we train the model for 3M steps under the same setting and report the result in Table 7. Under both training settings we observe performance advantage of SiT. We display more samples in Fig. 1 and in Appendix ??

Table 7: Benchmarking class-conditional image generation on ImageNet 256×256 and 512×512 . SiT-XL surpasses DiT-XL in both resolutions.

Class-Conditional Image	Net 2	56×25	56								
Model	FID↓	$\mathrm{sFID}\!\!\downarrow$	$\mathrm{IS}\uparrow$	Precision [↑]	$\operatorname{Recall}\uparrow$	Class-Conditional Image	Net 5	12×51	2		
BigGAN-deep [10] StyleGAN-XL [52]	6.95 2.30	7.36 4.02	171.4 265.12	0.87 0.78	0.28 0.53	Model	FID↓	sFID↓	IS↑	Precision↑	Recall↑
Mask-GIT [12]	6.18	-	182.1	-	-	BigGAN-deep [10] StyleGAN-XL [52]	8.43 2.41	8.13 4.06	$177.90 \\ 267.75$	0.88 0.77	0.29 0.52
ADM [19] ADM-G, ADM-U	10.94 3.94	6.02 6.14	100.98 215.84	0.69 0.83	0.63 0.53	Mask-GIT [12]	7.32	-	156.0	-	-
CDM [25]	4.88	-	158.71	-	-	ADM [19] ADM-G. ADM-U	23.24 3.85	$10.19 \\ 5.86$	58.06 221.72	0.73 0.84	$0.60 \\ 0.53$
RIN [30]	3.42	-	182.0	-	-	Simple Diffusion(U-Net) [27]	4.28	-	171.0	-	-
Simple Diffusion(U-Net) [27]	3.76	-	171.6	-	-	Simple Diffusion(U-ViT, L)	4.53	-	205.3	-	-
Simple Diffusion(U-ViT, L)	2.77	-	211.8	-	-	VDM++ [33]	2.65	-	278.1	-	-
VDM++ [33]	2.12	-	267.7	-	-	DiT-XL(cfg = 1.5) [45]	3.04	5.02	240.82	0.84	0.54
DiT-XL(cfg = 1.5) [45]	2.27	4.60	278.24	0.83	0.57	$\frac{1}{\text{SiT-XL}(cfg = 1.5, \text{SDE})}$	2.62	4 18	252.21	0.84	0.57
SiT-XL(cfg = 1.5, ODE) SiT-XL(cfg = 1.5, SDE)	2.15 2.06	4.60 4.49	258.09 277.50	0.81 0.83	0.60 0.59			1.10	202.21	0.01	0.01

4 Related Work

Transformers. The transformer architecture [62] has emerged as a powerful tool for application domains as diverse as vision [20, 44], language [63, 64], quantum chemistry [22], active matter systems [9], and biology [11]. Several works have built on DiT and have made improvements by modifying the architecture to internally include masked prediction layers [21, 65]; these choices are orthogonal to this work and may be fruitfully combined in future work.

Training and Sampling in Diffusions. Diffusion models arose from [24, 56, 59] and have close historical relationship with denoising methods [28, 29, 54]. Various

efforts have gone into improving the sampling algorithms behind these methods in the context of DDPM [57] and SBDM [32, 58]; these are also orthogonal to our studies and may be combined to push for better performance in future work. Improved Diffusion ODE [66] also studies several combinations of model parameterizations (velocity versus noise) and paths (VP versus Linear). Unlike our work, they focus on lower dimensional experiments, benchmark with likelihoods, and do not consider SDE sampling.

Interpolants and flow matching. Velocity parameterizations using the Linear interpolant were also studied in [38, 40], and were generalized to the manifold setting in [6]. A trade-off in bounds on the KL divergence between the target distribution and the model arises when considering sampling with SDEs versus ODE; [2] shows that minimizing the objectives presented in this work controls KL for SDEs, but not for ODEs. Error bounds for SDE-based sampling with score-based diffusion models are studied in [13, 14, 35, 36], for ODE-base sampling are explored in [7, 15], in addition to the Wasserstein bounds provided in [4].

Other related works make improvements by changing how noise and data are sampled during training. [47,60] compute mini-batch optimal couplings between the Gaussian and data distribution to reduce the transport cost and gradient variance; [3] instead build the coupling by flowing directly from the conditioning variable to the data for image-conditional tasks. Finally, various work considers learning a stochastic bridge connecting two arbitrary distributions [18,41,46,53]. These directions are compatible with our investigations; they specify the learning problem for which one can vary the choices of model parameterizations, interpolant schedules, and sampling algorithms.

Diffusion in Latent Space. Generative modeling in latent space [48, 61] is a tractable approach for modeling high-dimensional data. The approach has been applied beyond images to video generation [8], which is a yet-to-be explored and promising application area for velocity trained models. [17] also train velocity models in the latent space of the pre-trained Stable Diffusion VAE. They demonstrate promising results for the DiT-B backbone with a final FID-50K of 4.46; their study was one motivation for the investigation in this work regarding which aspects of these models contribute to the gains in performance over DiT.

5 Conclusion

In this work, we have presented Scalable Interpolant Transformers, a simple and powerful framework for image generation tasks. Within the framework, we explored the tradeoffs between a number of key design choices: the choice of a continuous or discrete-time model, the choice of interpolant, the choice of model prediction, and the choice of diffusion coefficient. We highlighted the advantages and disadvantages of each choice and demonstrated how careful decisions can lead to significant performance improvements. Many concurrent works [23,31,39,42] explore similar approaches in a wide variety of downstream tasks, and we leave the application of SiT to these tasks for future works.

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