

Appa: Bending weather dynamics with latent diffusion models

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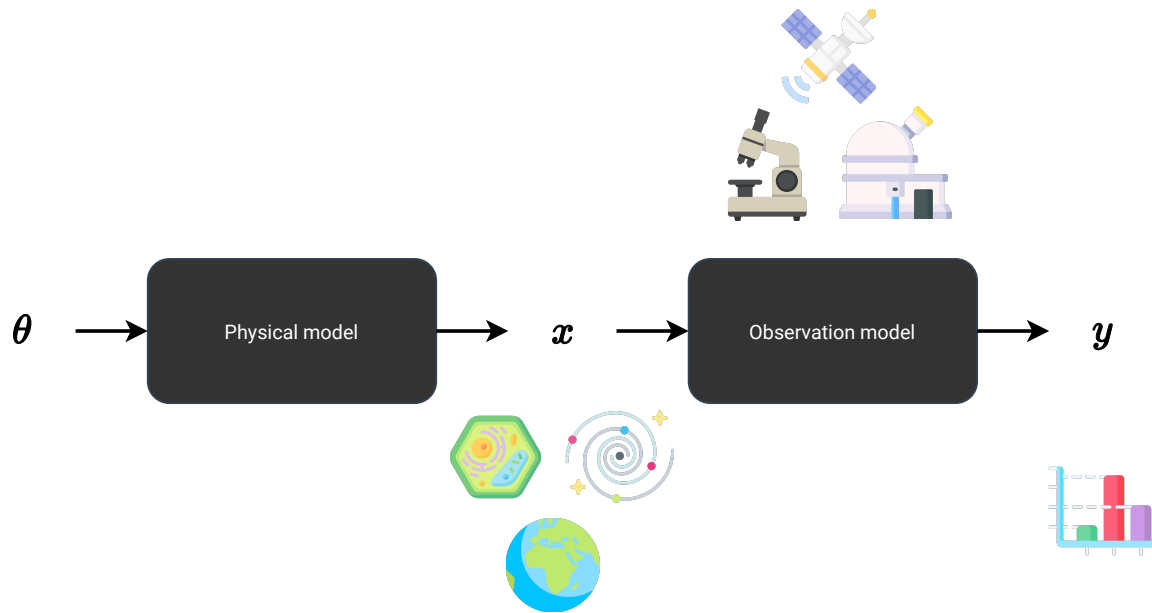
From a noisy observation y ...

**... can we recover
all plausible images x ?**

$$\dot{u} = -u \nabla u + \frac{1}{Re} \nabla^2 u - \frac{1}{\rho} \nabla p + f$$

$$0 = \nabla \cdot u$$

... or parameters $\theta = \{Re, \rho, f\}$?

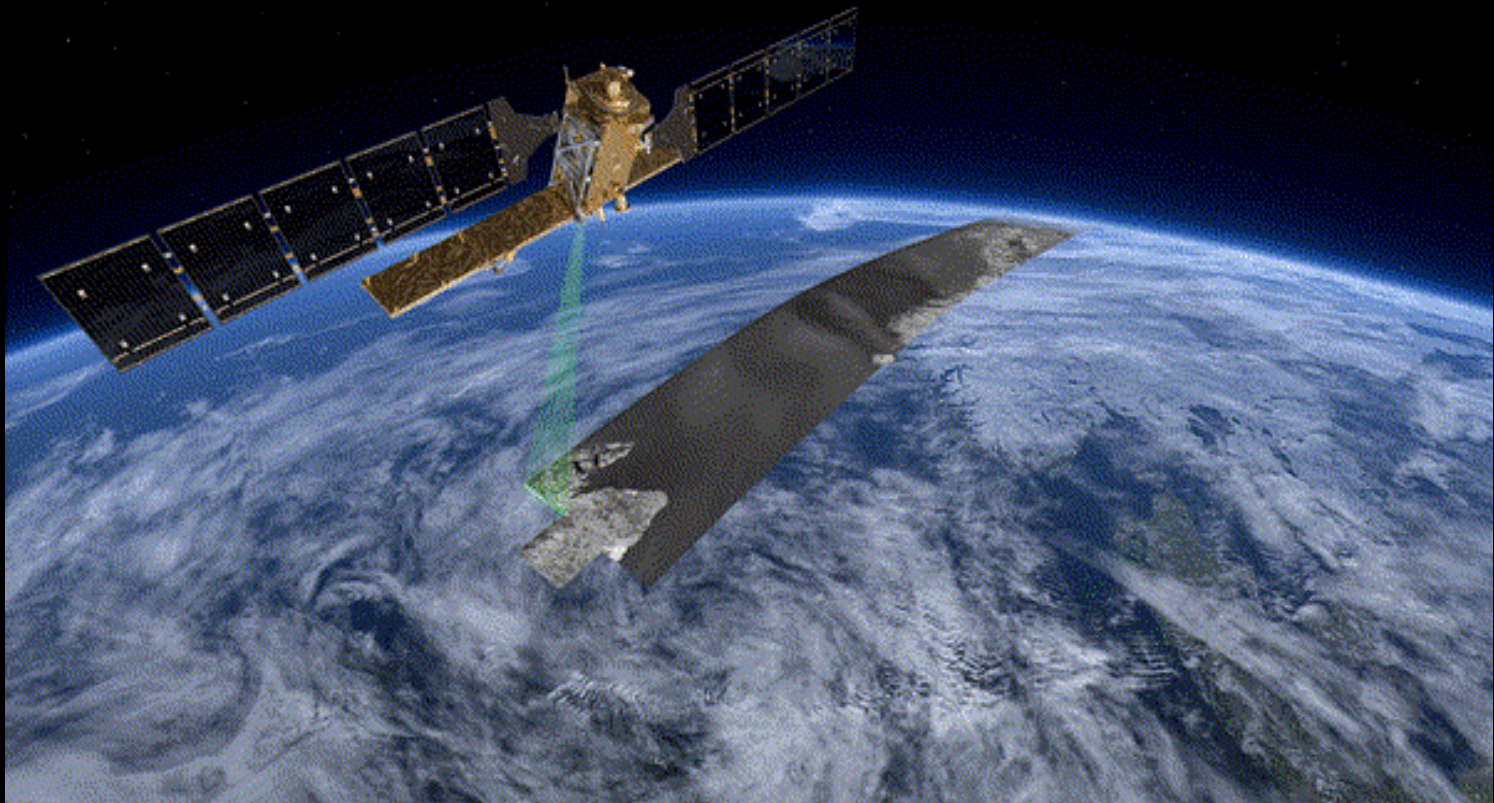


Bayesian inverse problems

Given a noisy observation y , estimate either

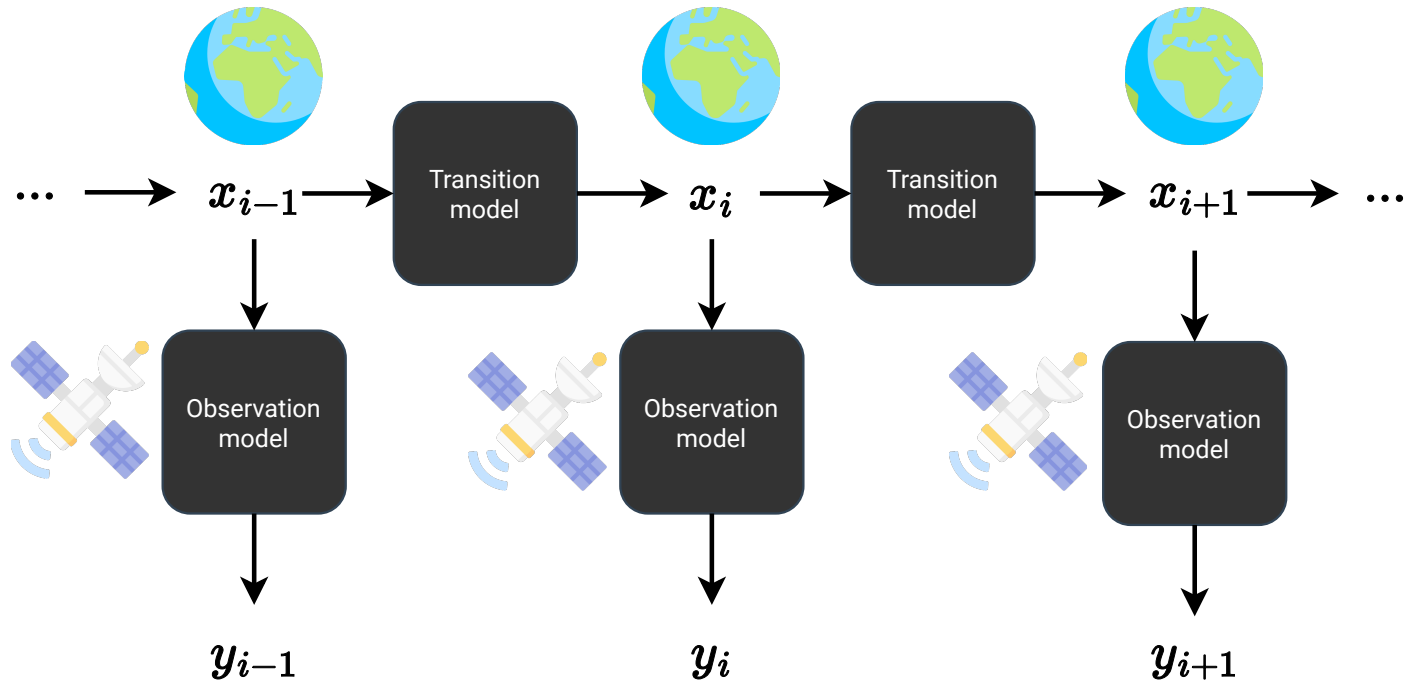
- the posterior distribution $p(x|y) \propto p(x)p(y|x)$ of latent states x , or
- the posterior distribution $p(\theta|y)$ of parameters θ ,

assuming a prior $p(\theta)$ and forward models $p(x|\theta)$ and $p(y|x)$.



Today: from a sequence noisy observations $\mathbf{y}_{1:L}$ (e.g., from satellites),
can we recover past and present atmospheric states $\mathbf{x}_{1:L}$?

Data assimilation



The goal of **data assimilation** is to estimate plausible trajectories $x_{1:L}$ given one or more noisy observations y (or $y_{1:L}$) as the posterior

$$p(x_{1:L}|y) = \frac{p(y|x_{1:L})}{p(y)} p(x_0) \prod_{i=1}^{L-1} p(x_{i+1}|x_i).$$

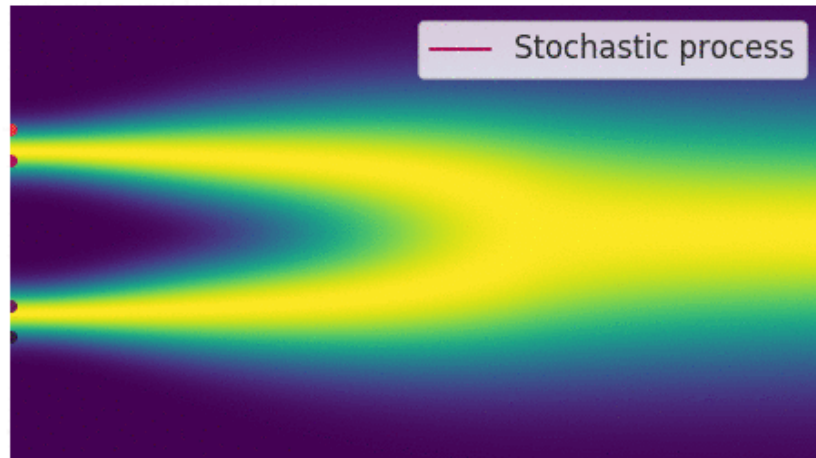
Diffusion models for inverse problems

Diffusion models 101

Samples $x \sim p(x)$ are progressively perturbed through a diffusion process described by the forward SDE

$$dx_t = f_t x_t dt + g_t dw_t,$$

where x_t is the perturbed sample at time t .

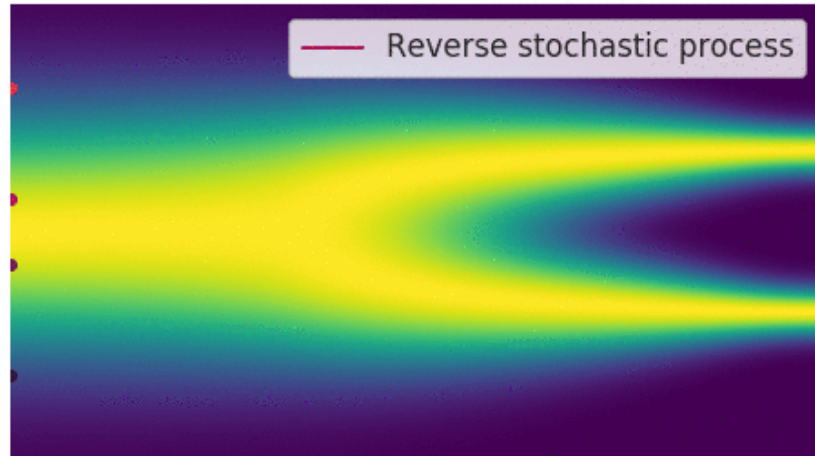


Forward diffusion process.

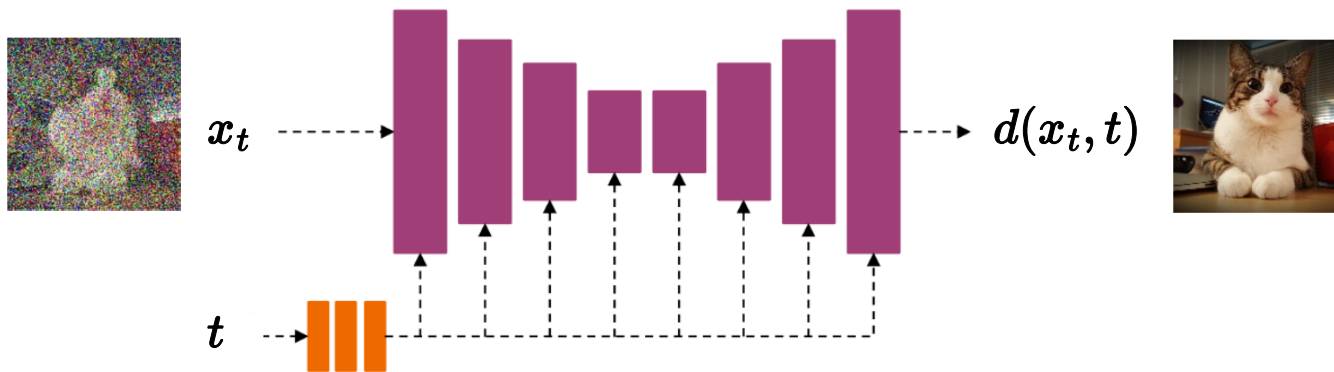
The reverse process satisfies a reverse-time SDE that can be derived analytically from the forward SDE as

$$dx_t = [f_t x_t - g_t^2 \nabla_{x_t} \log p(x_t)] dt + g_t dw_t.$$

Therefore, to generate data samples $x_0 \sim p(x_0) \approx p(x)$, we can draw noise samples $x_1 \sim p(x_1) \approx \mathcal{N}(0, \Sigma_1)$ and gradually remove the noise therein by simulating the reverse SDE from $t = 1$ to 0 .



Reverse denoising process.



The score function $\nabla_{x_t} \log p(x_t)$ is unknown, but can be approximated by a neural network $d_\theta(x_t, t)$ by minimizing the denoising score matching objective

$$\mathbb{E}_{p(x)p(t)p(x_t|x)} [\|d_\theta(x_t, t) - x\|_2^2].$$

The optimal denoiser d_θ is the mean $\mathbb{E}[x|x_t]$ which, via Tweedie's formula, relates to the score function as

$$\nabla_{x_t} \log p(x_t) \approx \Sigma_t^{-1} (d_\theta(x_t, t) - x_t).$$

Inverting an observation

Let's assume an observation $y \sim p(y|x)$ for some unknown latent state x .

To turn a diffusion model $p_\theta(x)$ into a conditional model $p_\theta(x|y)$, we can add conditioning information y at each step of the reverse process by adding y as an additional input to the denoiser $d_\theta(x_t, t, y)$.



Using the Bayes' rule, the posterior score $\nabla_{x_t} \log p(x_t|y)$ to inject in the reverse SDE can be decomposed as

$$\nabla_{x_t} \log p(x_t|y) = \nabla_{x_t} \log p(x_t) + \nabla_{x_t} \log p(y|x_t) - \nabla_{x_t} \log p(y).$$

This enables **zero-shot posterior sampling** from a diffusion prior $p(x_0)$ without having to pre-wire the denoiser to the observation model $p(y|x)$.



Approximating $\nabla_{x_t} \log p(y|x_t)$

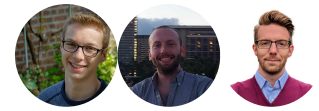
We want to estimate the score $\nabla_{x_t} \log p(y|x_t)$ of the noise-perturbed likelihood

$$p(y|x_t) = \int p(y|x)p(x|x_t)dx.$$

Our approach:

- Assume a linear Gaussian observation model $p(y|x) = \mathcal{N}(y|Ax, \Sigma_y)$.
- Assume the approximation $p(x|x_t) \approx \mathcal{N}(x|\mathbb{E}[x|x_t], \mathbb{V}[x|x_t])$, where $\mathbb{E}[x|x_t]$ is estimated by the denoiser and $\mathbb{V}[x|x_t]$ is estimated using Tweedie's covariance formula.
- Then $p(y|x_t) \approx \mathcal{N}(y|A\mathbb{E}[x|x_t], \Sigma_y + A\mathbb{V}[x|x_t]A^T)$.
- The score $\nabla_{x_t} \log p(y|x_t)$ then approximates to

$$\nabla_{x_t} \mathbb{E}[x|x_t]^T A^T (\Sigma_y + A\mathbb{V}[x|x_t]A^T)^{-1} (y - A\mathbb{E}[x|x_t]).$$

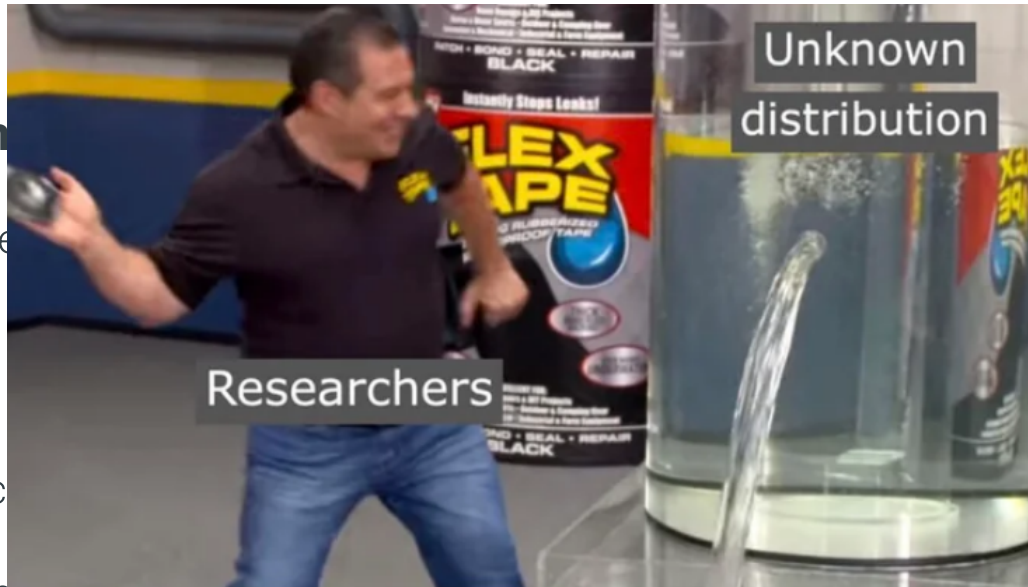


Approxim

We want to e

Our approach

- Assume
- Assume $\mathbb{E}[x|x_t]$
Tweedie
- Then $p(\dots)$
- The sco



Unknown distribution

Researchers

likelihood



Gaussian distribution

, Σ_y).

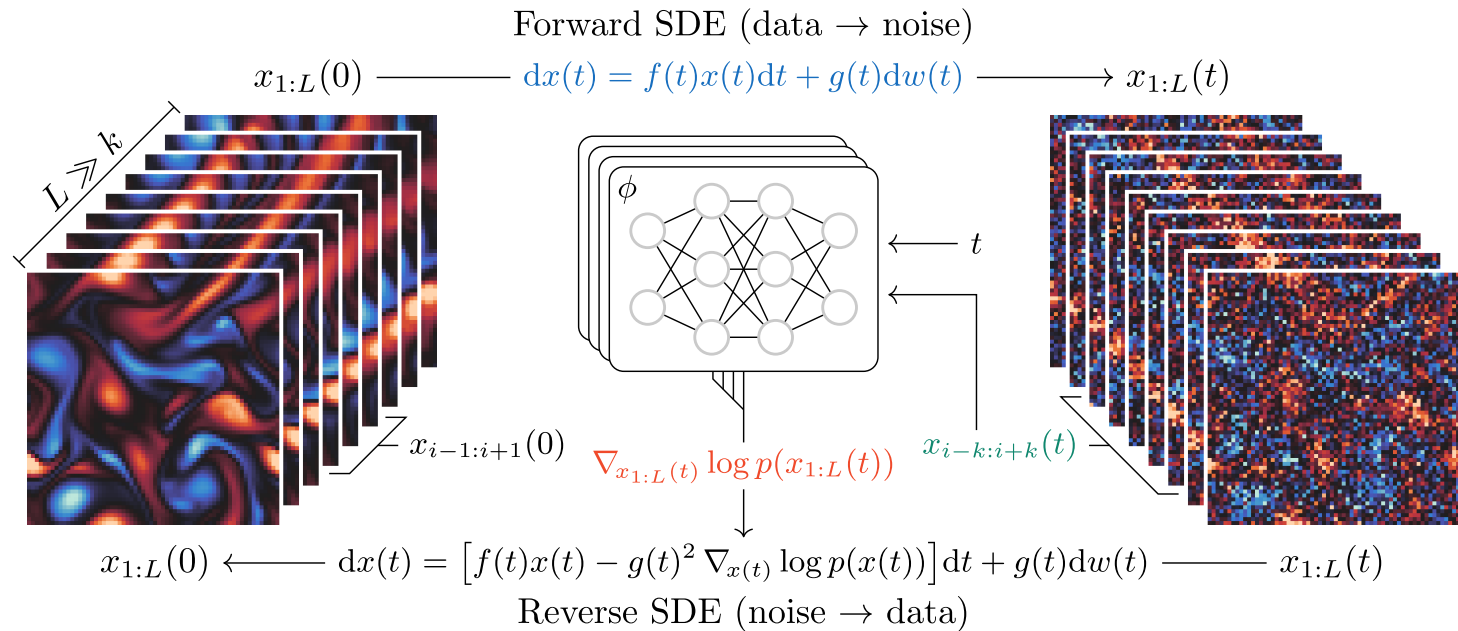
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Data assimilation with diffusion models

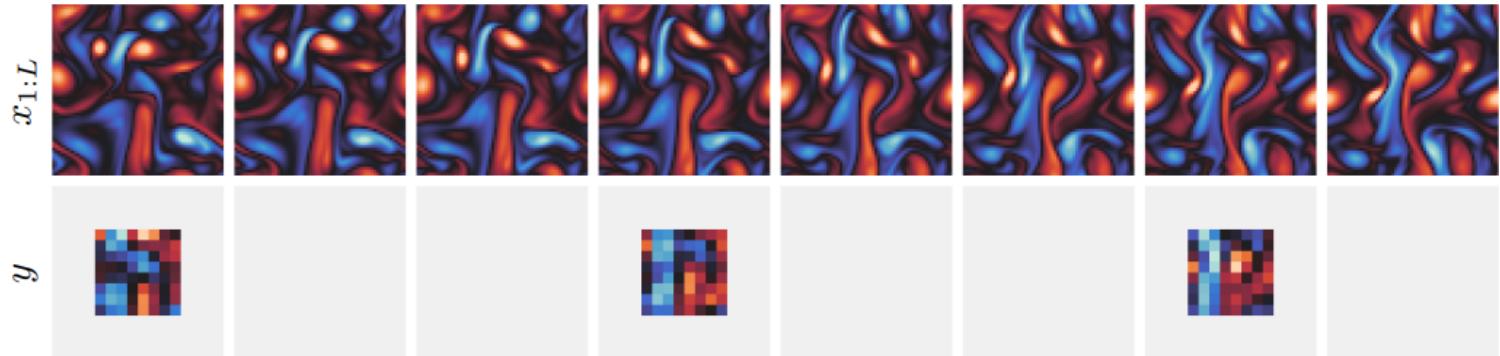


Score-based data assimilation (SDA)

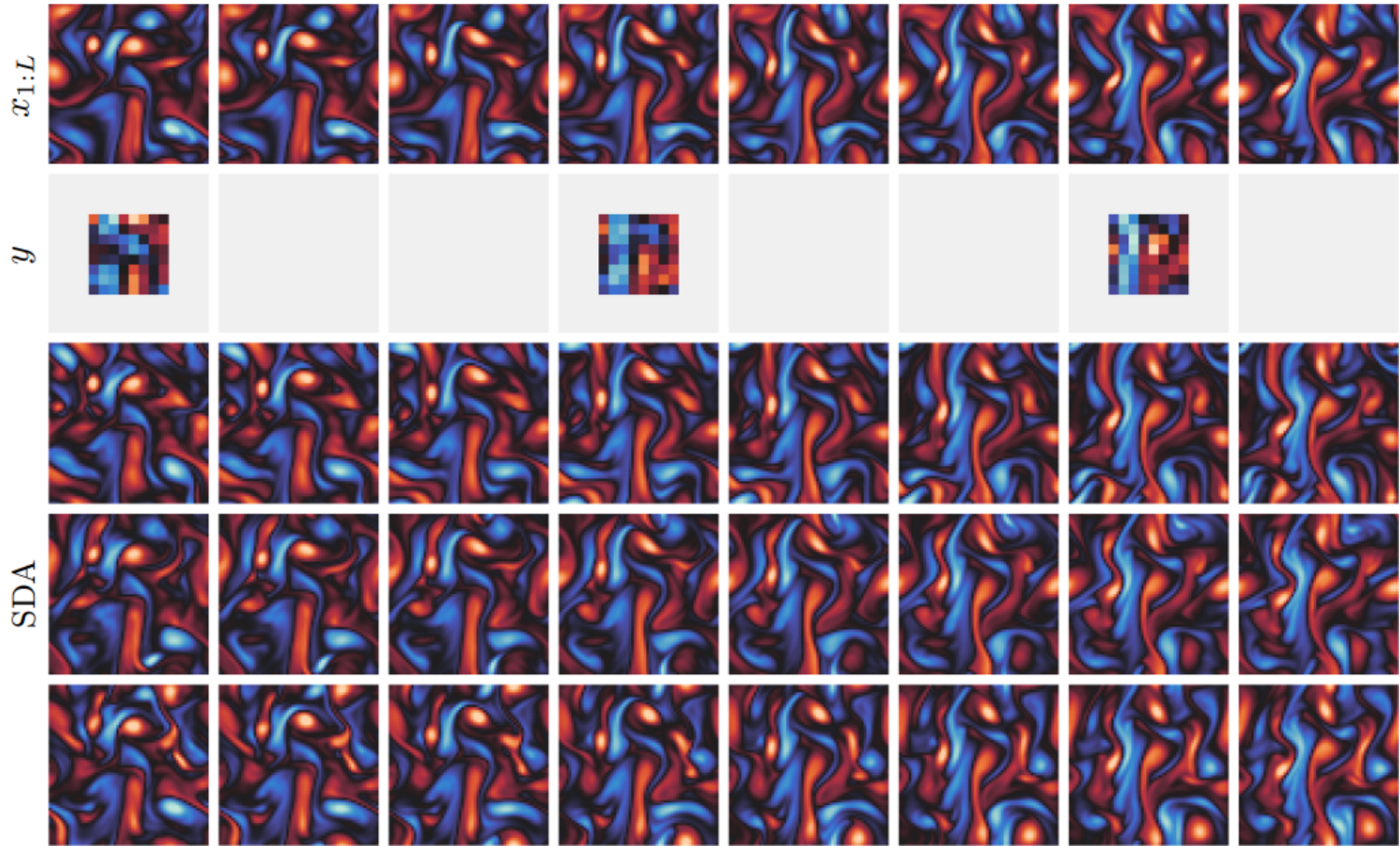


Our approach:

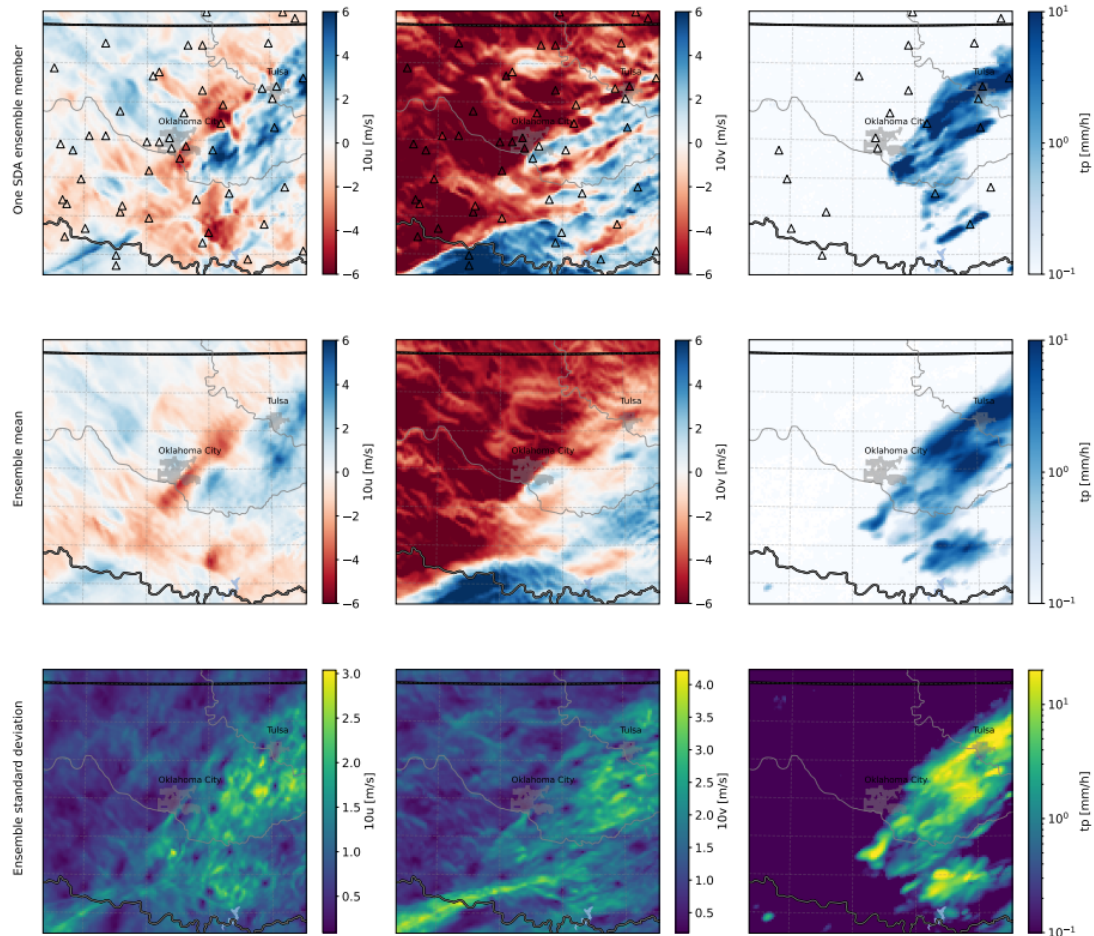
- Build a score-based generative model $p(x_{1:L})$ of arbitrary-length trajectories.
- Use zero-shot posterior sampling to generate plausible trajectories from noisy observations y .



Sampling trajectories $x_{1:L}$ from
noisy, incomplete and coarse-grained observations y .



Sampling trajectories $x_{1:L}$ from
noisy, incomplete and coarse-grained observations y .



SDA can assimilate noisy weather observations to produce stochastic ensembles at the regional scale.

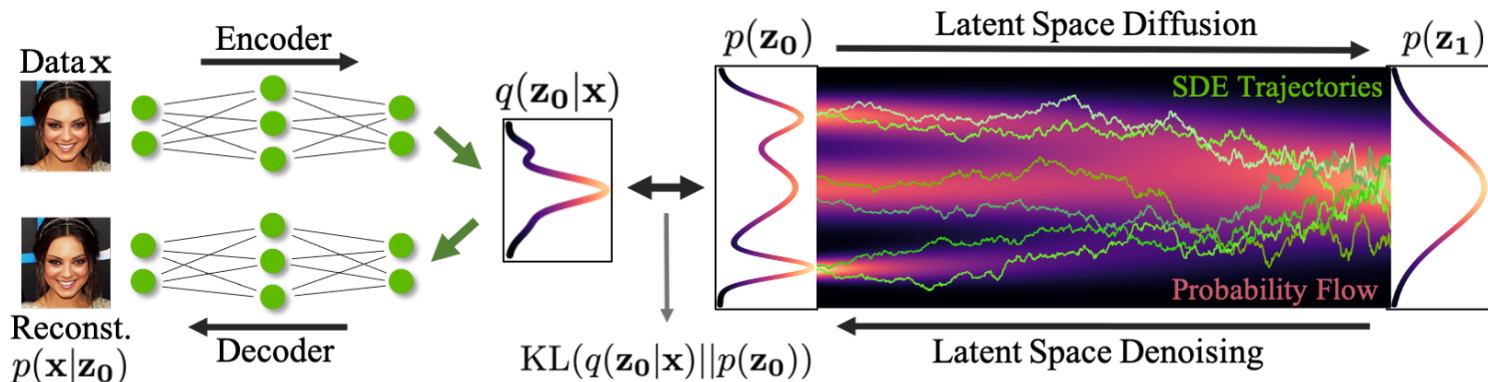


Scaling SDA to a high-resolution Earth model?

Latent diffusion models (LDMs)

Diffusion models scale to high-dimensional data by generating in the latent space of an autoencoder $x \approx D(E(x))$.

If x is the data and $z = E(x)$ is the latent representation produced by an encoder E , then the diffusion model generates $z \sim p_\theta(z)$ which is then decoded into $x = D(z)$ by a decoder D .

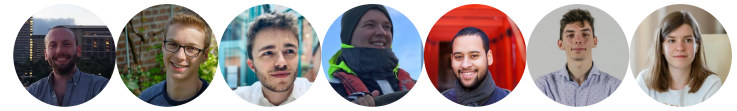


LDMs for inverse problems

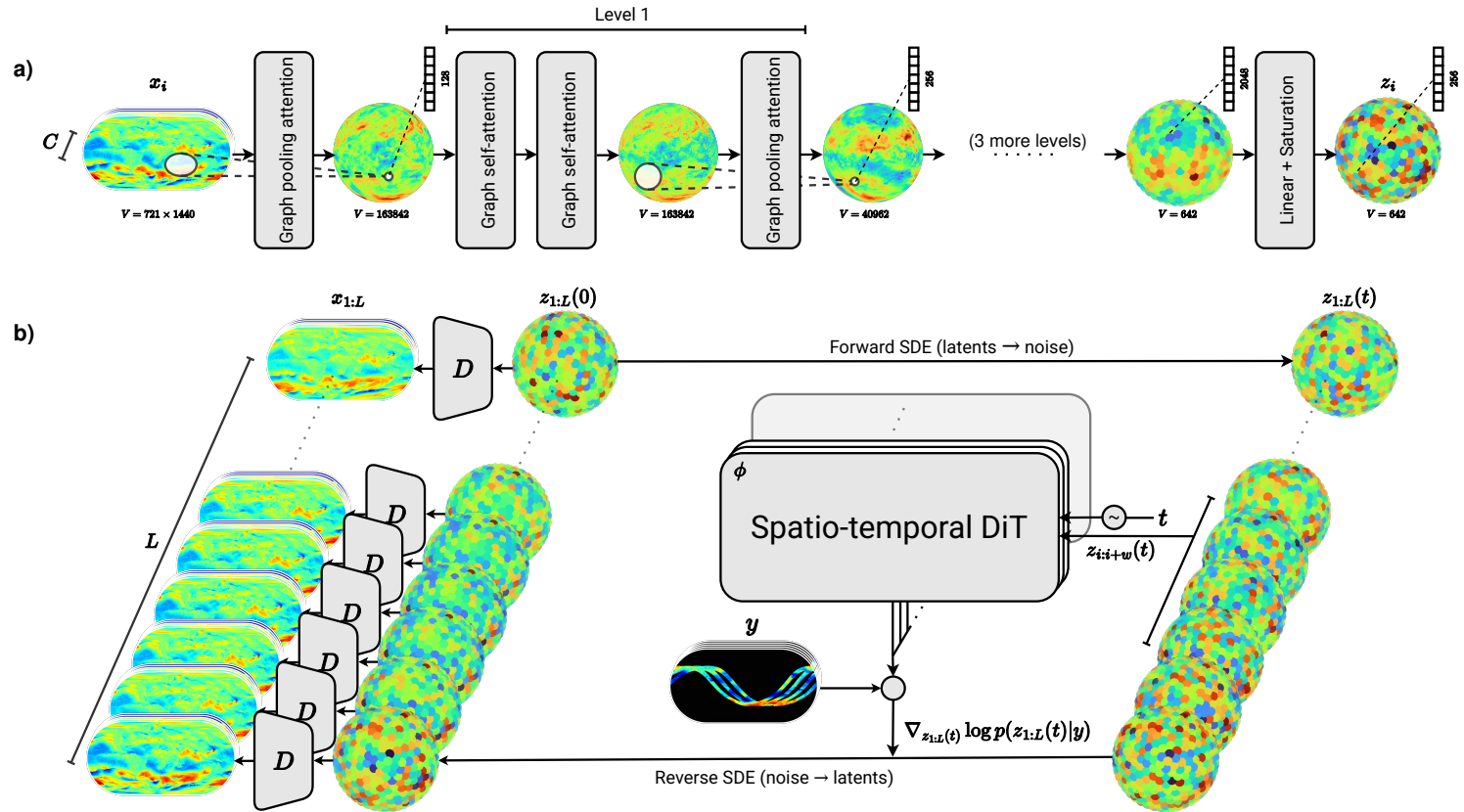
$$x \sim p_\theta(x|y) \Leftrightarrow z \sim p_\theta(z|y), x = D(z)$$

But how to sample from $p_\theta(z|y)$?

- If the observation model in data space is $p(y|x) = \mathcal{N}(y|M(x), \Sigma_y)$, then an observation model in the latent space can be defined as $p(y|z) = \mathcal{N}(y|M(D(z)), \Sigma_y)$.
- Regular posterior sampling algorithms can then be used to sample from the posterior distribution $p_\theta(z|y)$.



Appa: Bending weather dynamics with LDMs



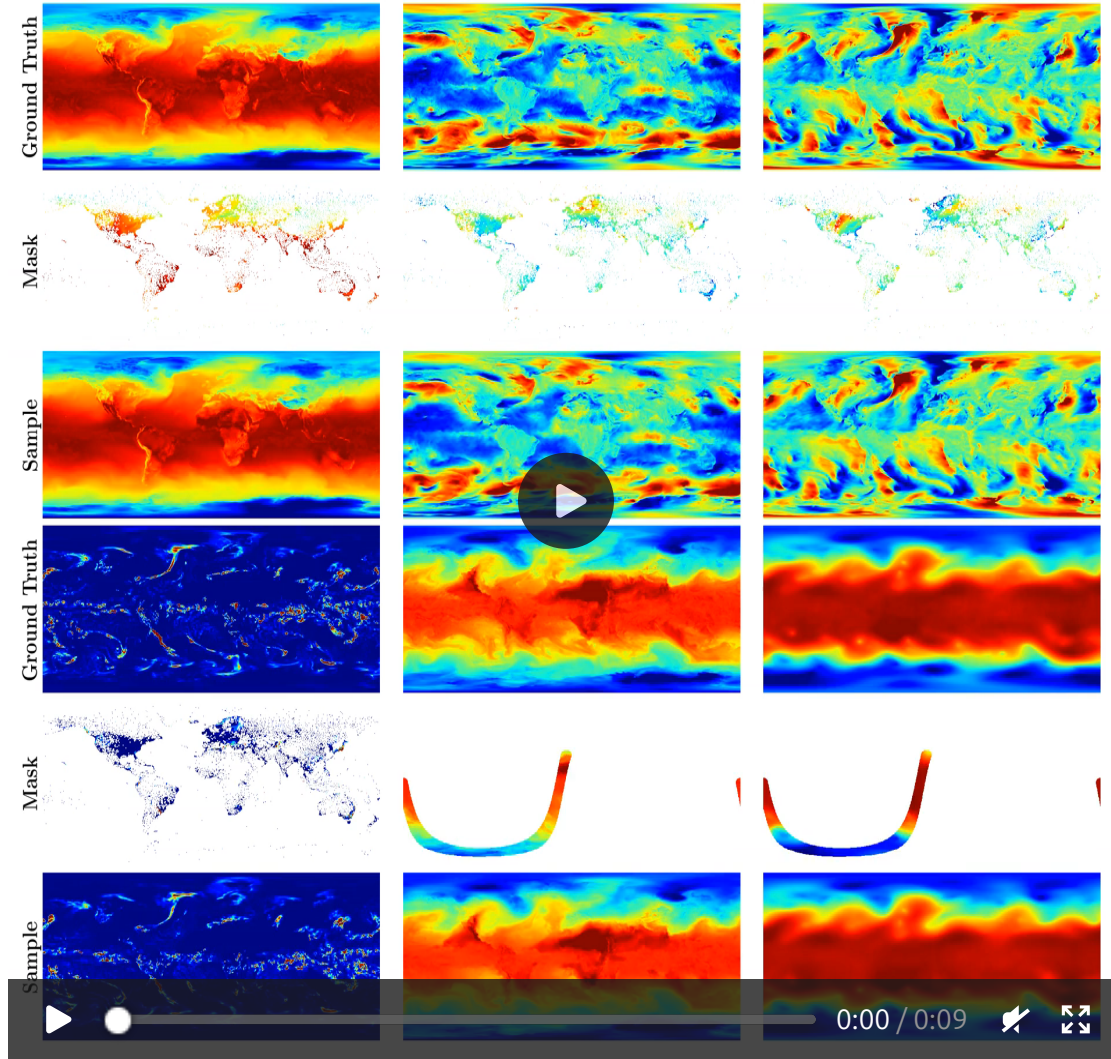
Appa is made of three components:

- a 500M-parameter **autoencoder** that compresses the data space x into a latent space z with a 450x compression factor;
- a 1B-parameter **diffusion model** that generates latent trajectories $z_{1:L}$;
- a zero-shot **posterior sampling algorithm** adapted from MMPS (Rozet et al, 2024) that samples from the posterior distribution $p(z_{1:L} | y)$.

Appa can solve multiple inverse problems **without retraining**:

- reanalysis of past atmospheric states $p(\mathbf{x}_{1:L}|\mathbf{y}_{1:L})$;
- filtering of the present atmospheric state $p(\mathbf{x}_L|\mathbf{y}_{1:L})$;
- forecasting of future atmospheric states $p(\mathbf{x}_{L+1:L+M}|\mathbf{y}_{1:L})$ or $p(\mathbf{x}_{L+1:L+M}|\mathbf{x}_L)$.

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Reanalysis of past data $p(x_{1:L}|y_{1:L})$.

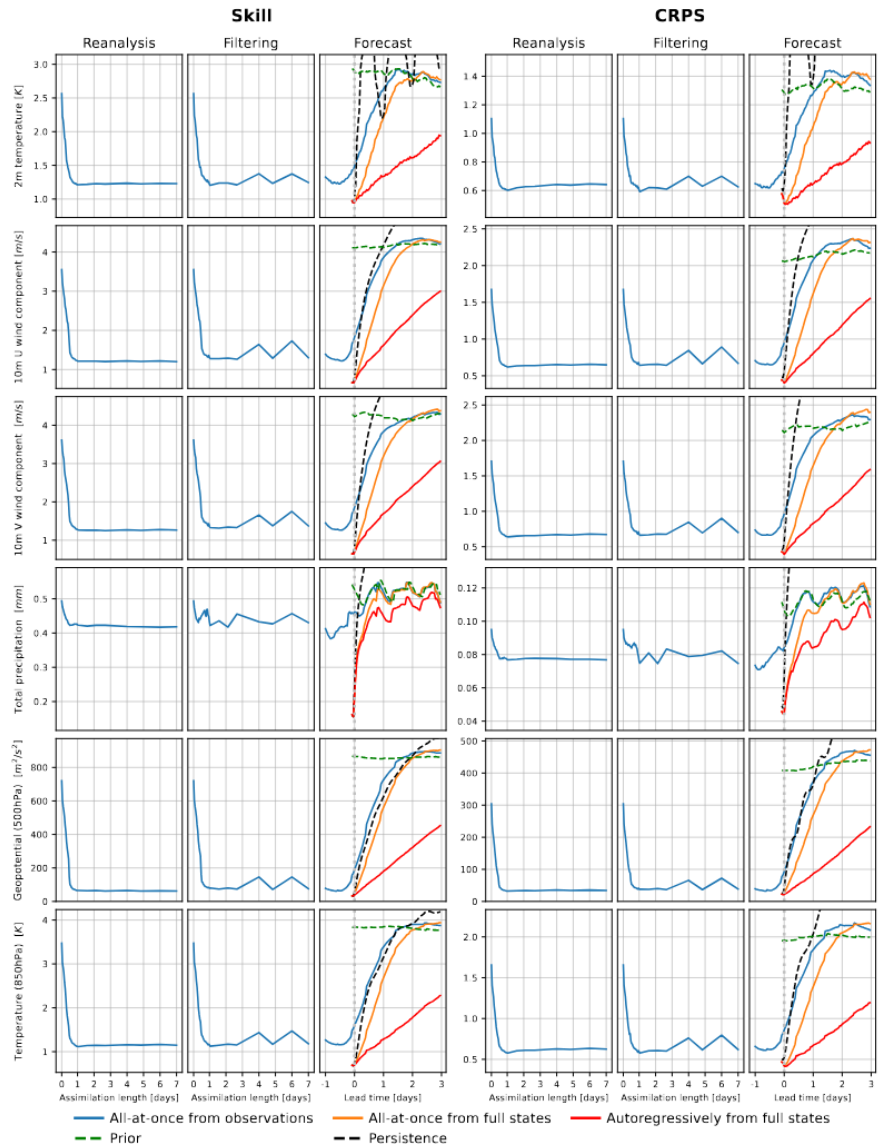


Forecasting of future data $p(x_{L+1:L+M} | y_{1:L})$.



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Unconditional sampling of (long) trajectories $p(\mathbf{x}_{1:L})$.





Conclusions

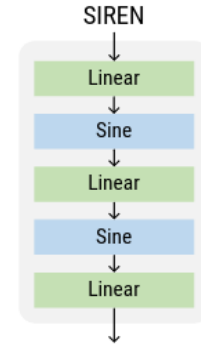
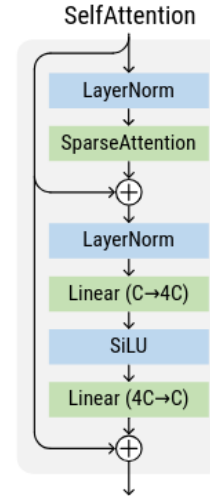
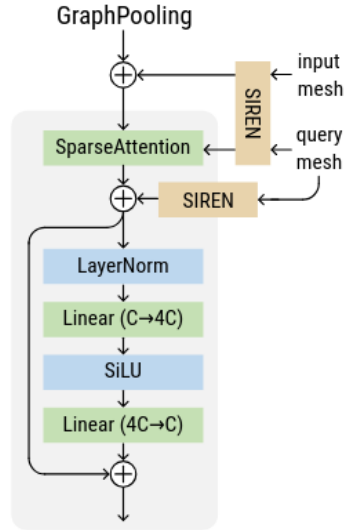
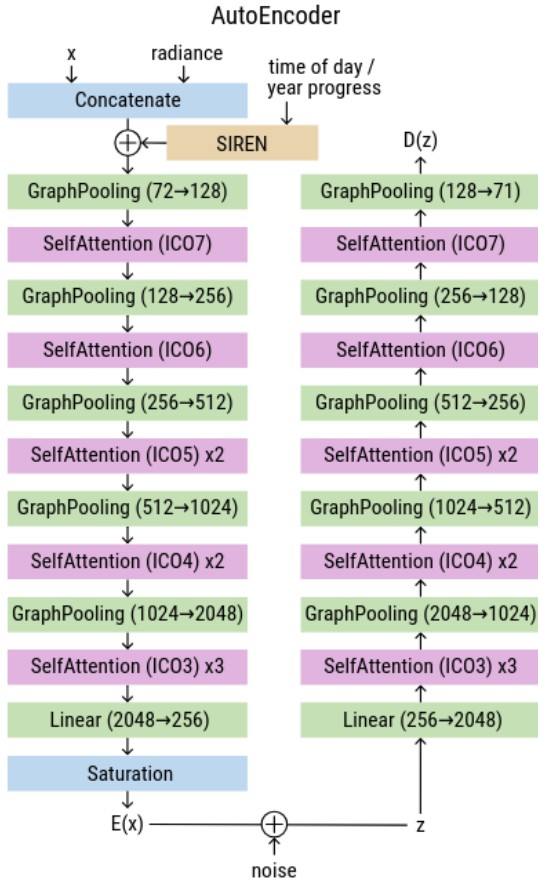
Score-based generative models...

- can be used for high-dimensional inverse problems;
- enable zero-shot posterior sampling, without pre-wiring the network to observations.

Appa...

- is a large weather model that offers a new perspective on data assimilation;
- can be used for reanalysis, filtering and forecasting;
- shows good results for reanalysis and filtering, moderate forecasting skills (for now!).

Appa: Autoencoder



Appa: Latent denoiser

