

Inverting scientific images with deep generative models

AI for Science seminar
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From a noisy observation y ...

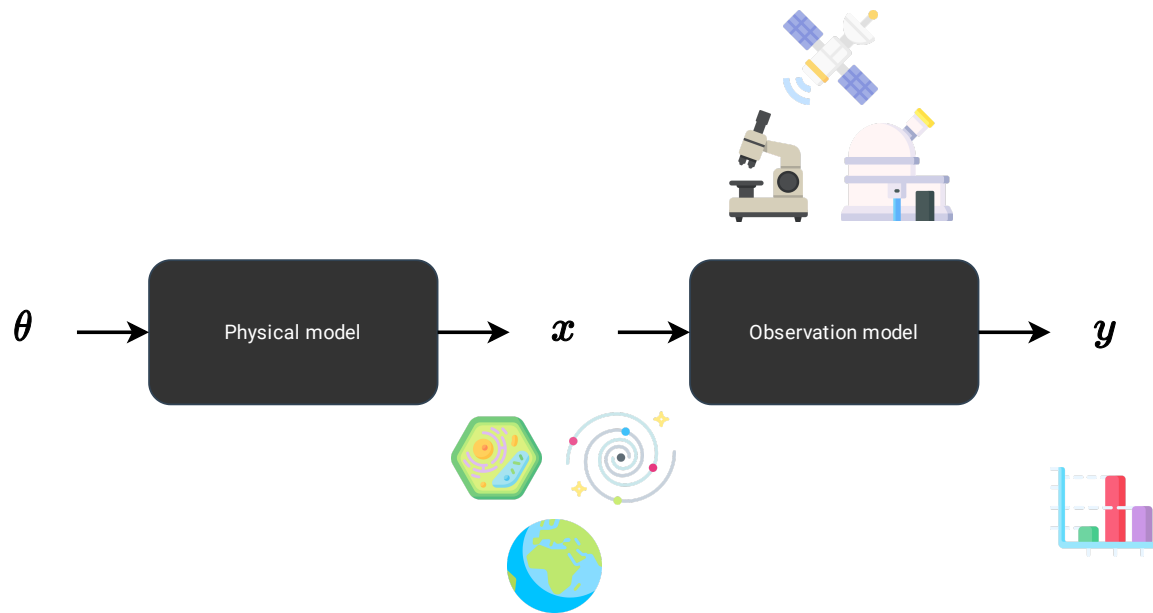
**... can we recover
all plausible states x ?**

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

$$0 = \nabla \cdot u$$

... or model parameters

$$\theta = \{Re, \rho, f\}?$$



Inverse problems in science

Given noisy observations 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 model parameters θ .

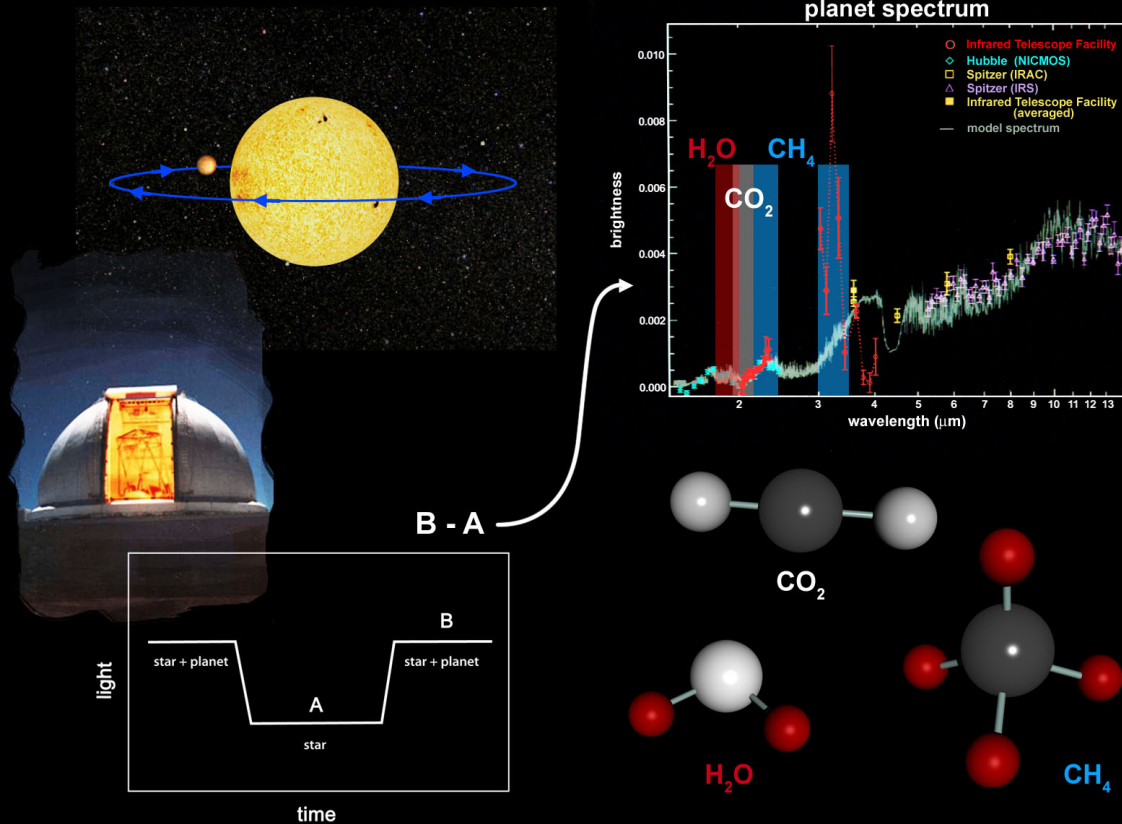


Part 1: Low-dimensional inverse problems

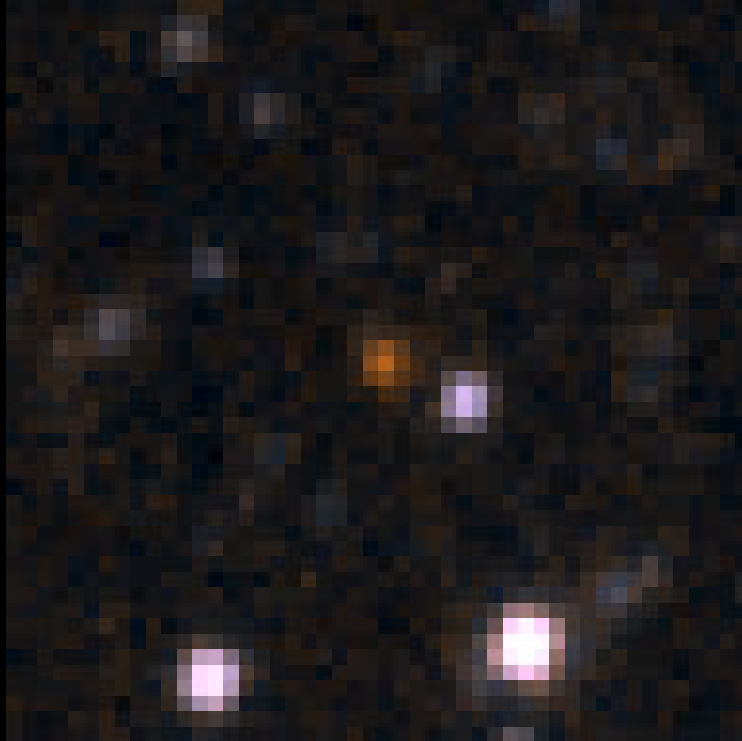
$p(\theta|x)$, with $\theta \in \mathbb{R}^d$, $d = O(10)$.



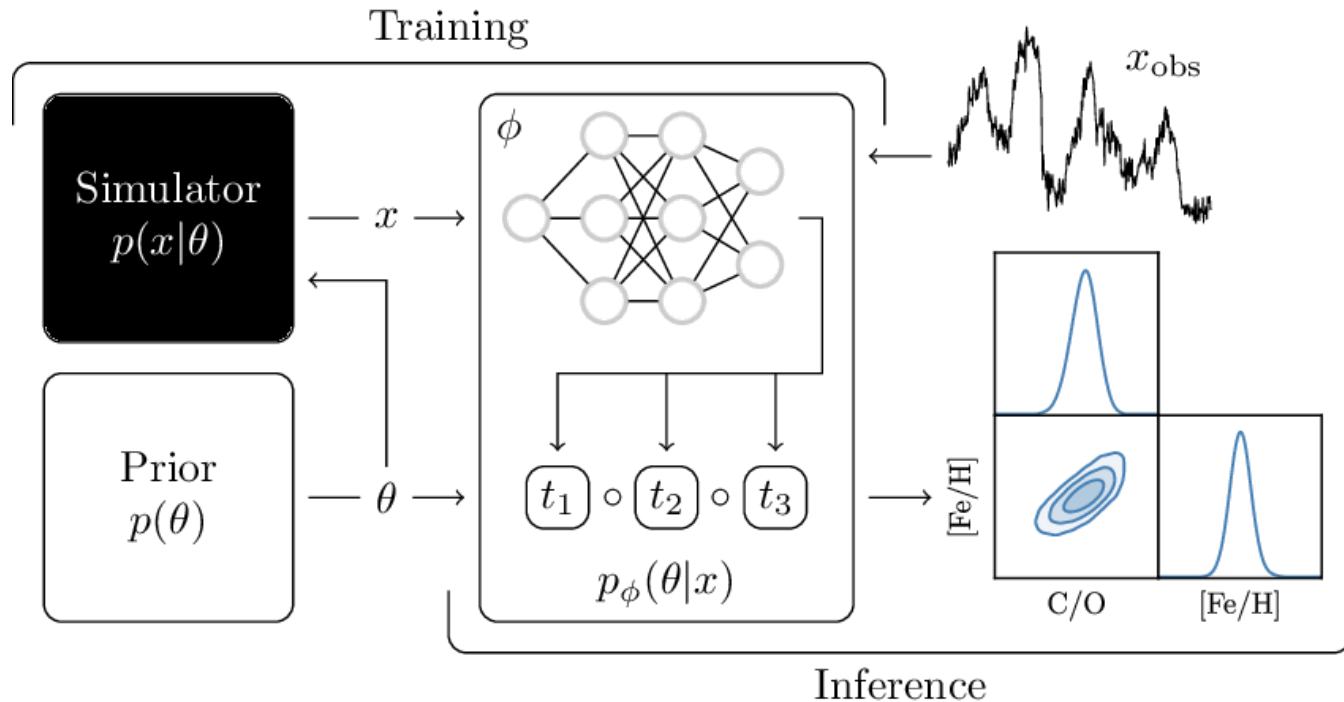
Exoplanet atmosphere characterization



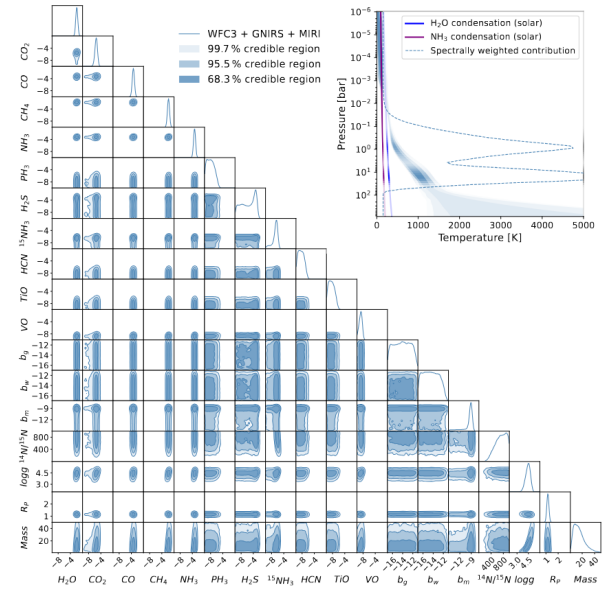
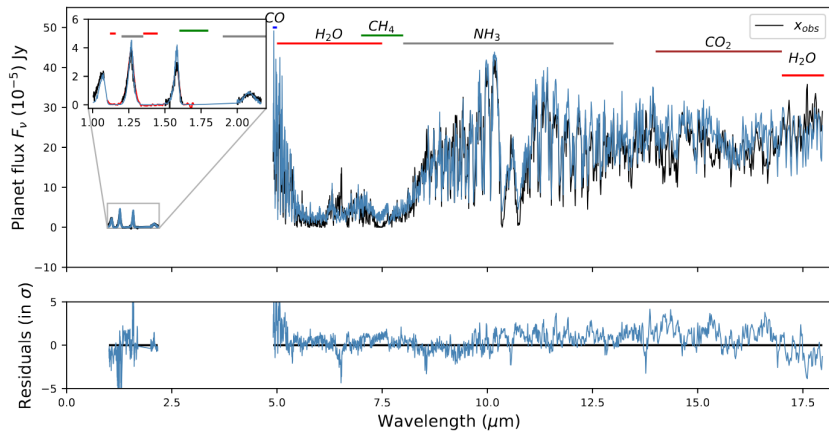
What are the atmospheres of exoplanets made of?
How do they form and evolve? Do they host life?



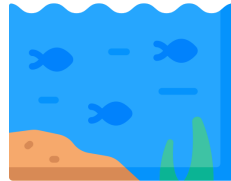
WISE 1738+2732, a brown dwarf 25 light-years away.



Using **Neural Posterior Estimation** (NPE), we approximate the posterior distribution $p(\theta|x)$ of atmospheric parameters θ with a **normalizing flow** trained on pairs (θ, x) simulated from a physical model of exoplanet atmospheres.



Panchromatic characterization of WISE 1738+2732 using JWST/MIRI.



Part 2: Large inverse problems

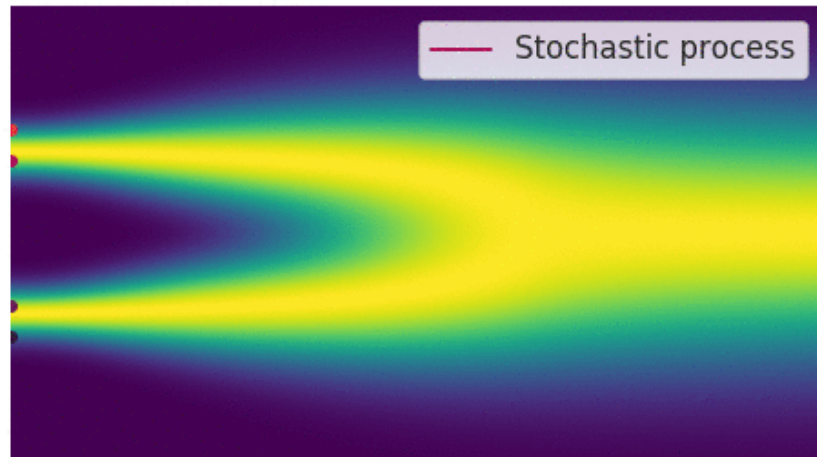
$p(x|y)$, with $x \in \mathbb{R}^d$, $d = O(10^5)$.

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 .

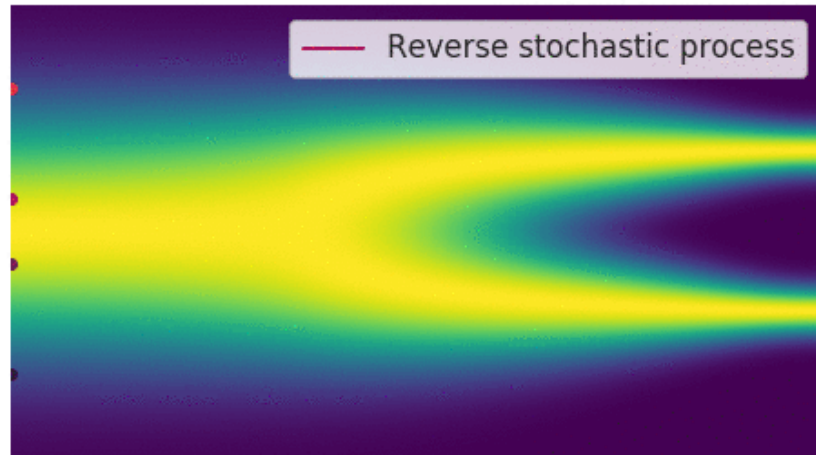


Forward diffusion process.

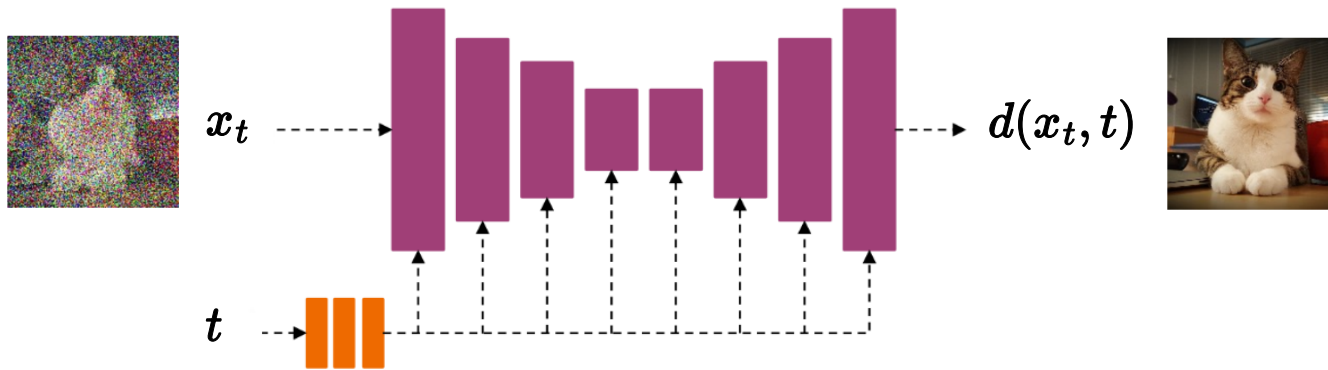
The reverse process satisfies a reverse-time SDE that can be derived analytically from the forward SDE as

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

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, allows to use

$$s_\theta(x_t, t) = \Sigma_t^{-1} (d_\theta(x_t, t) - x_t)$$

as a score estimate of $\nabla_{x_t} \log p(x_t)$ in the reverse SDE.

Inverting single observations

To turn a diffusion model $p_\theta(\mathbf{x})$ into a conditional model $p_\theta(\mathbf{x}|\mathbf{y})$, we can **hard-wire** conditioning information \mathbf{y} as an additional input to the denoiser $d_\theta(x_t, t, \mathbf{y})$ and train the model on pairs (x, \mathbf{y}) .



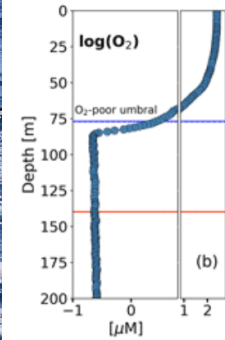
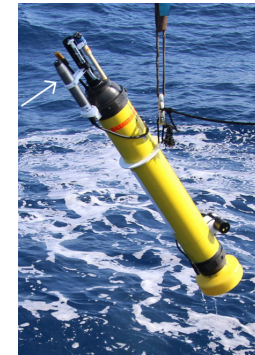
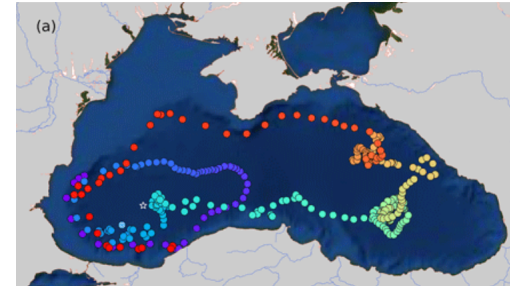
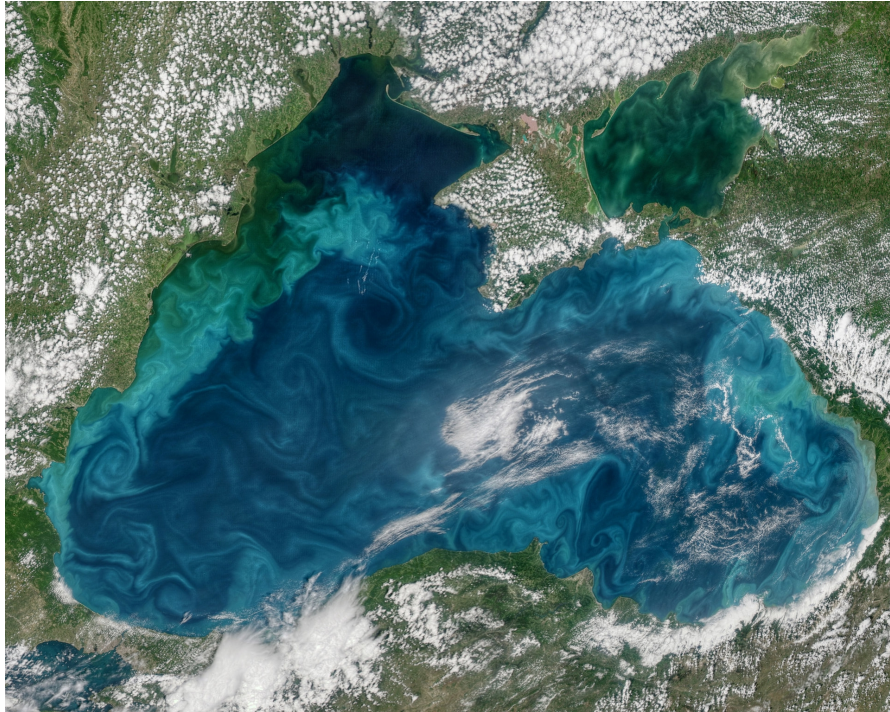
Using the Bayes' rule, the posterior score $\nabla_{x_t} \log p(x_t | y)$ to inject in the reverse SDE can be decomposed as

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

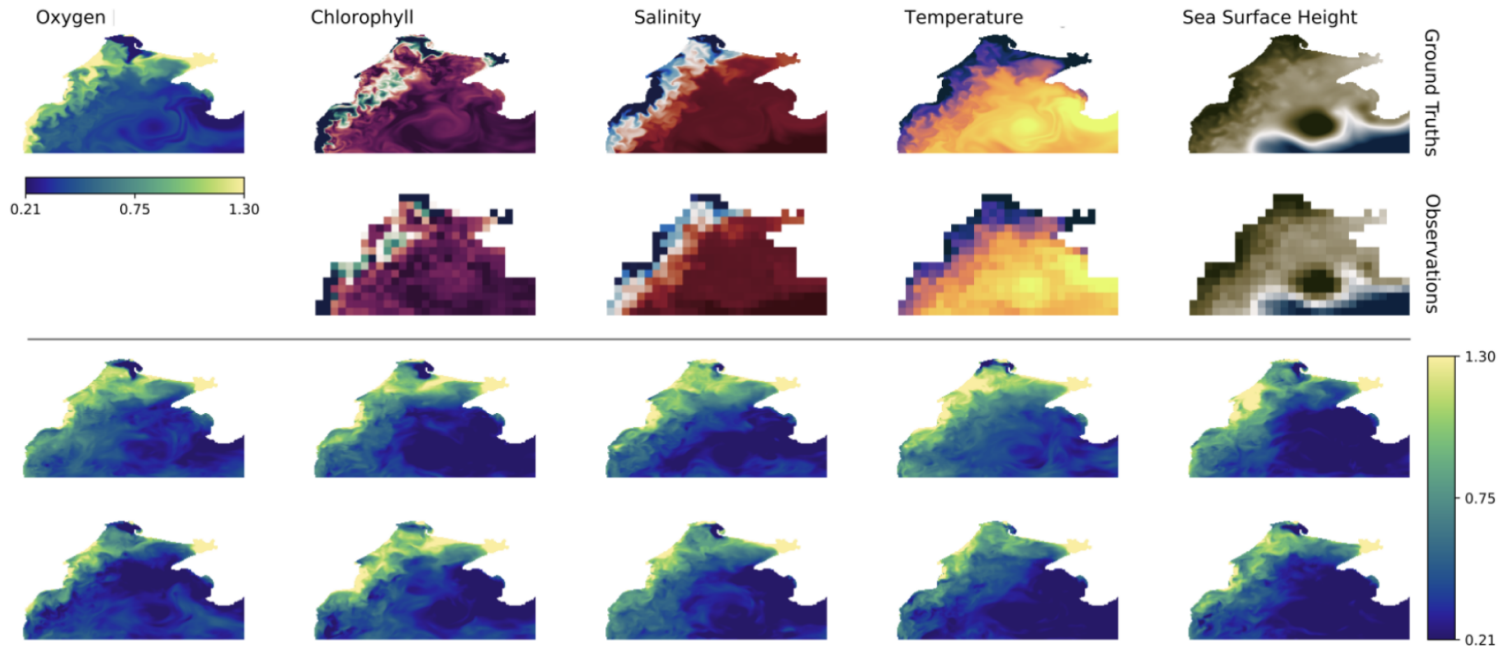
This enables **zero-shot posterior sampling** from a diffusion prior $p(x_0)$ without having to hard-wire the neural denoiser to the observation model $p(y | x)$.



Nowcasting Black Sea hypoxia from satellite observations



How do hypoxic zones evolve in response to climate change? Can we monitor them from space or with sparse measurements?

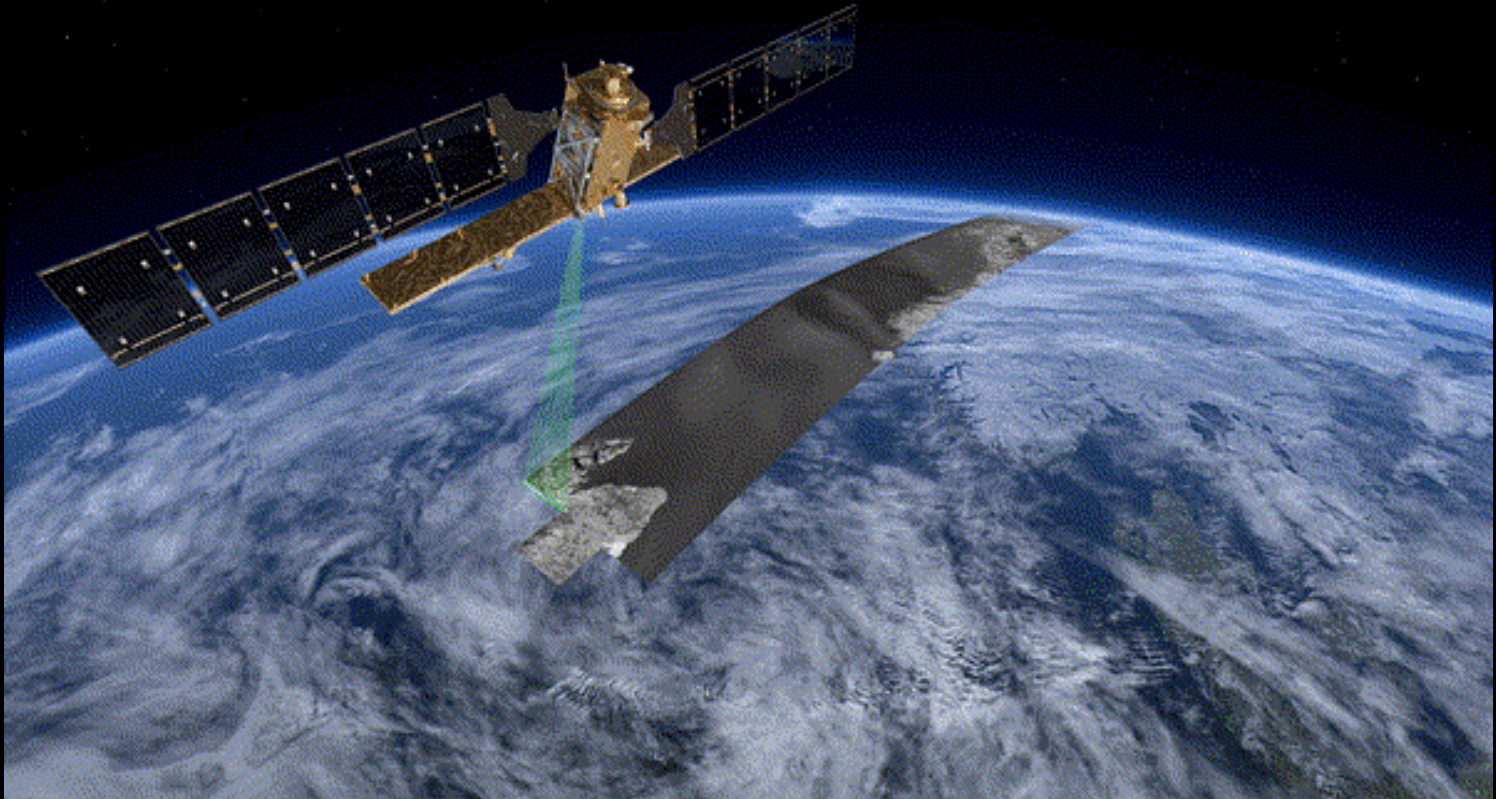


Posterior oxygen maps $p(x|y)$ can be recovered from satellite observations y of the surface, by zero-shot posterior sampling from a diffusion prior $p(x)$ of the Black Sea dynamics.

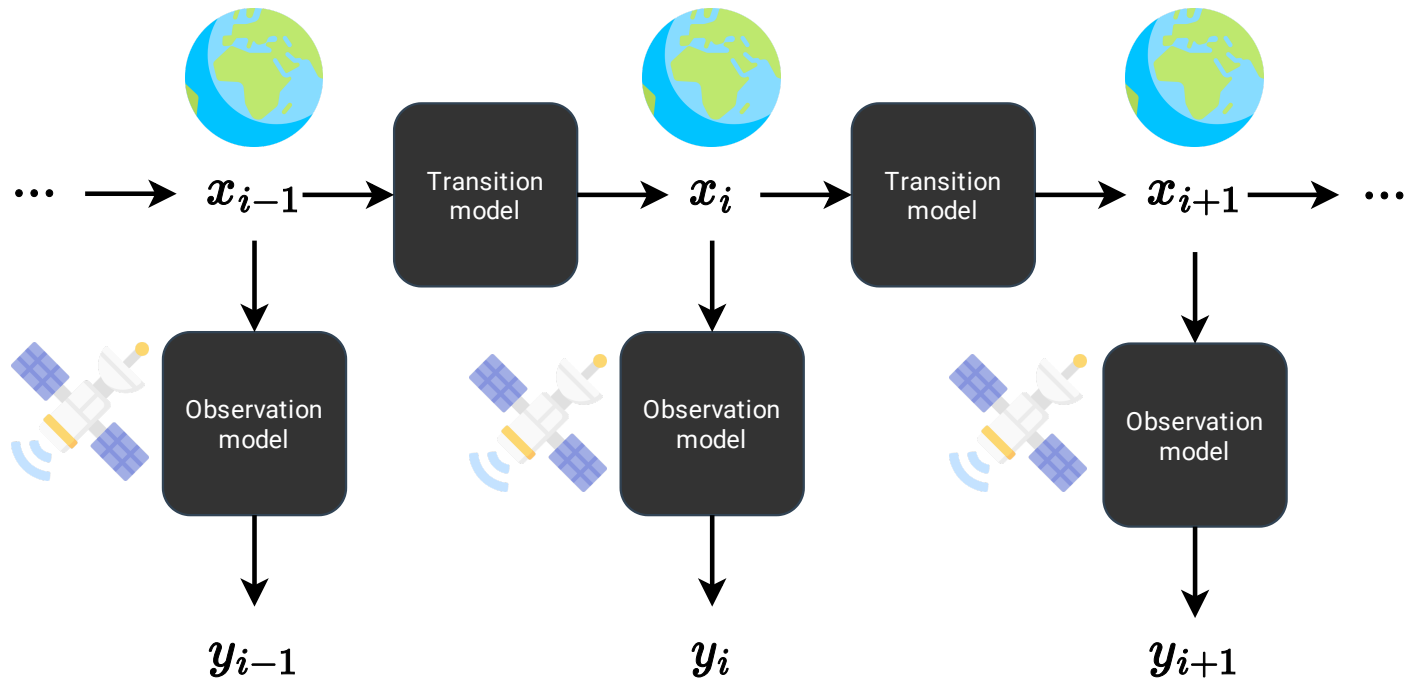


Part 3: Extra-large inverse problems

$p(x|y)$, with $x \in \mathbb{R}^d$, $d = O(10^6 +)$.

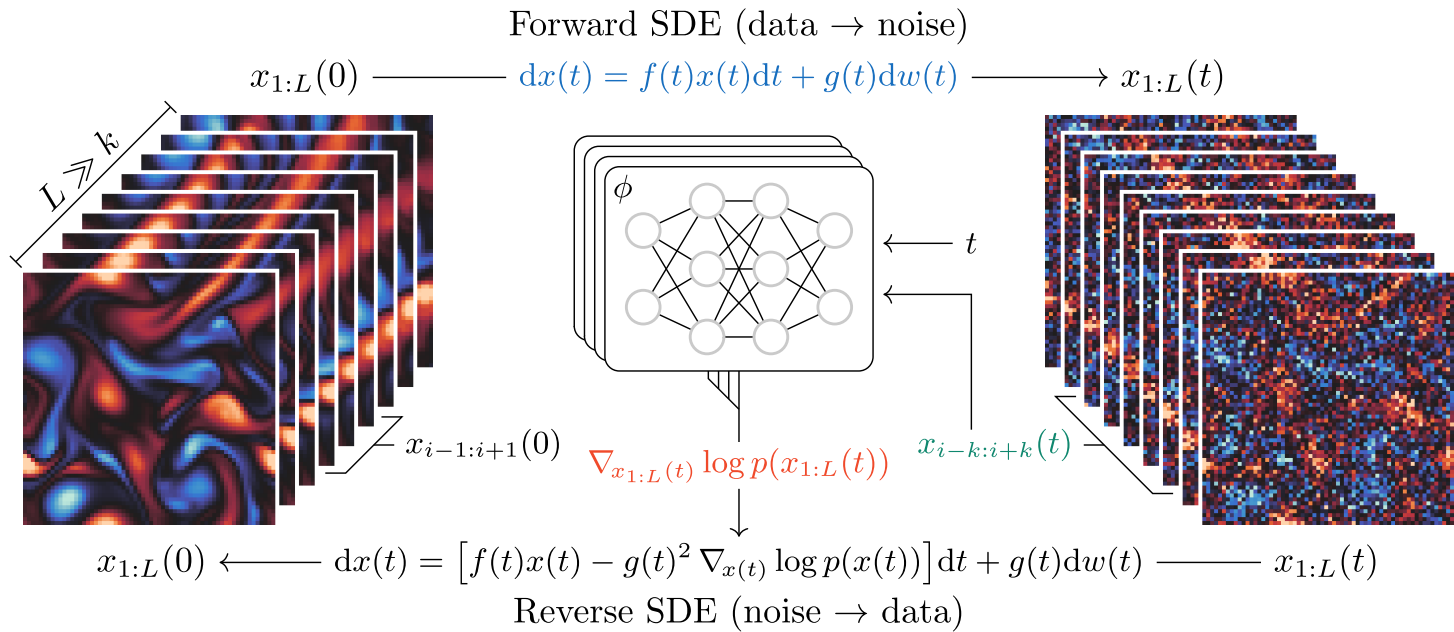


How can we create a comprehensive record of Earth's atmospheric evolution to understand climate change and improve weather prediction?



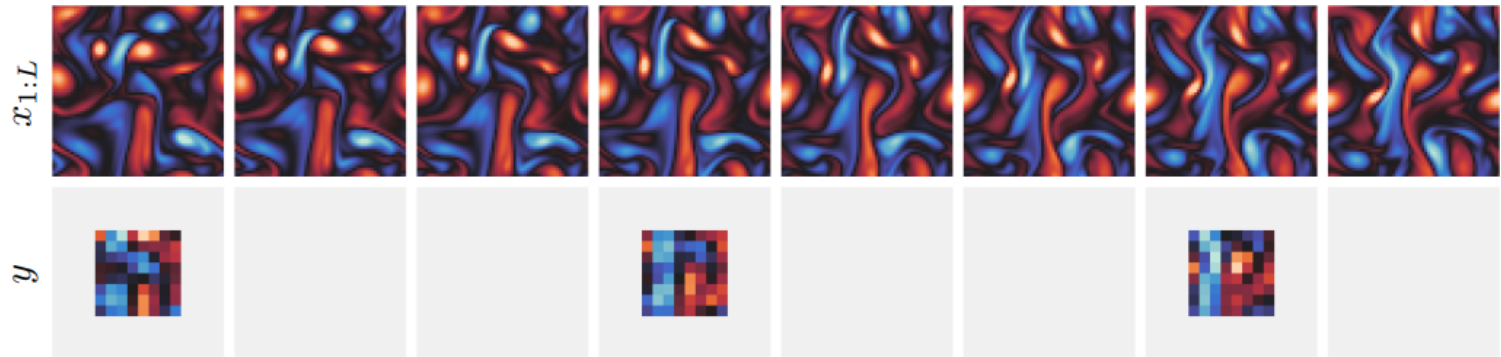
The goal of **data assimilation** is to estimate plausible trajectories $x_{1:L}$ given one or more noisy observations y (or $y_{1:L}$) as the posterior

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

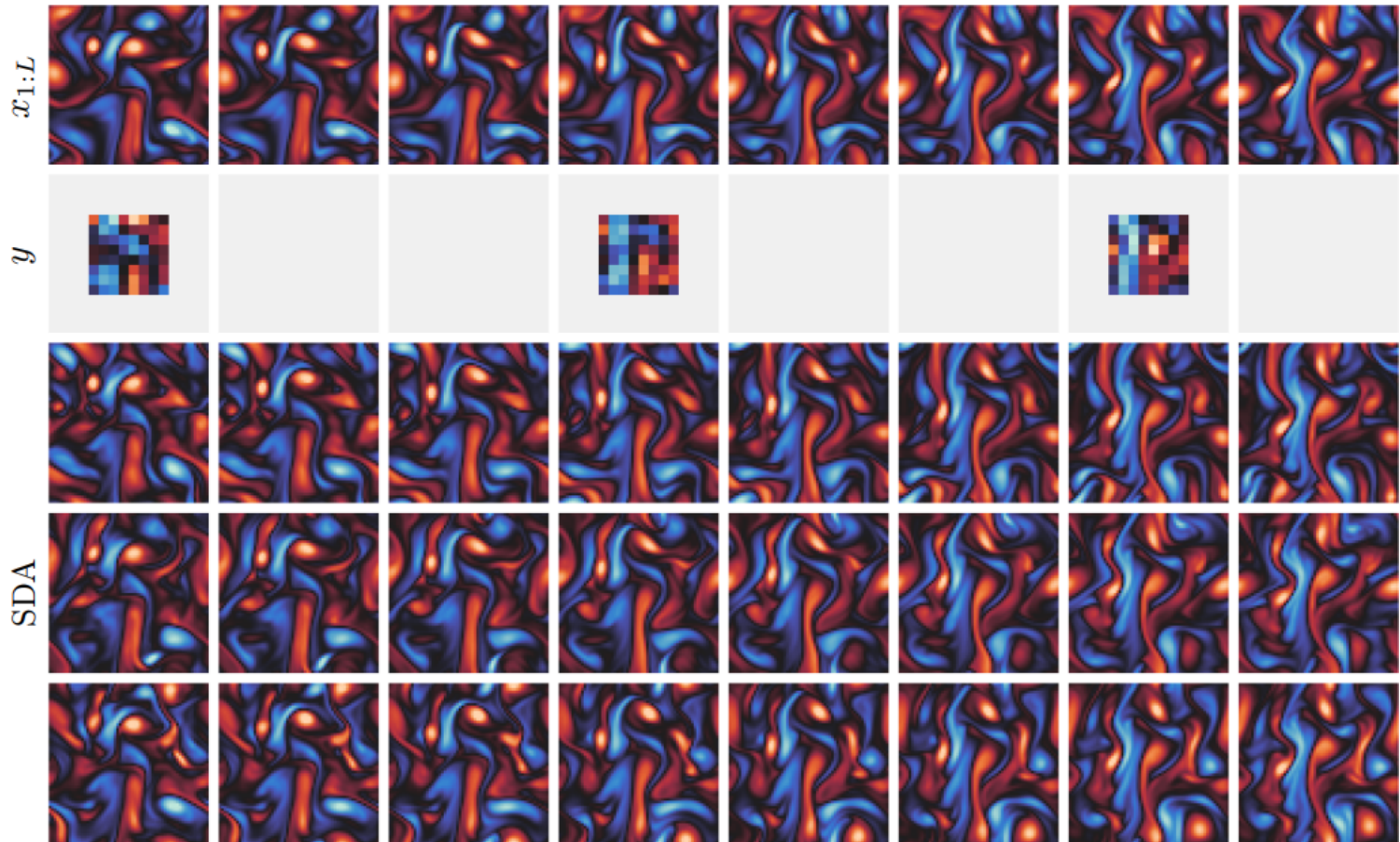


Score-based data assimilation

- 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 .



... but does it scale to a whole Earth model?

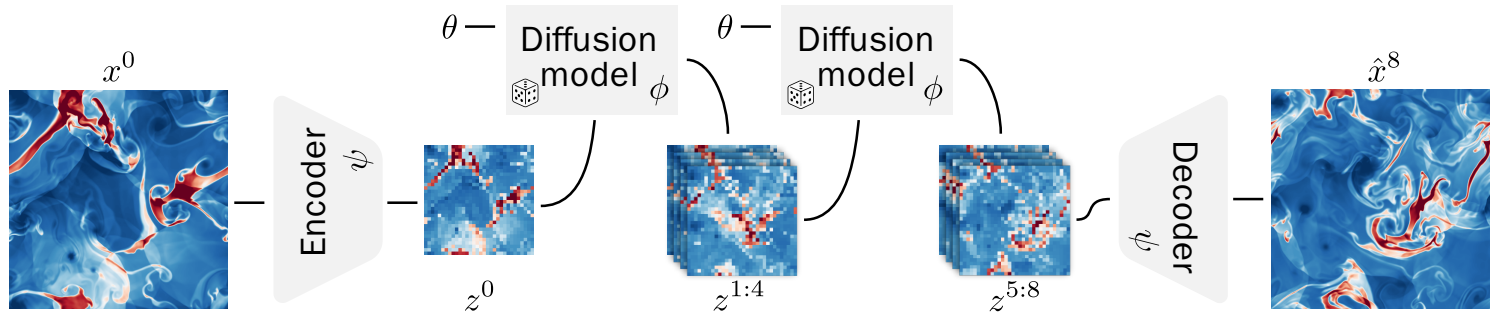
At 0.25° resolution, for 6 atmospheric variables, 13 pressure levels, hourly time steps, and 14 days of simulation, a trajectory $x_{1:L}$ contains $721 \times 1440 \times 6 \times 13 \times 24 \times 14 = 27 \times 10^9$ variables.



$O(10^9)$ variables (or more) is needed to capture the complexity of the atmosphere.

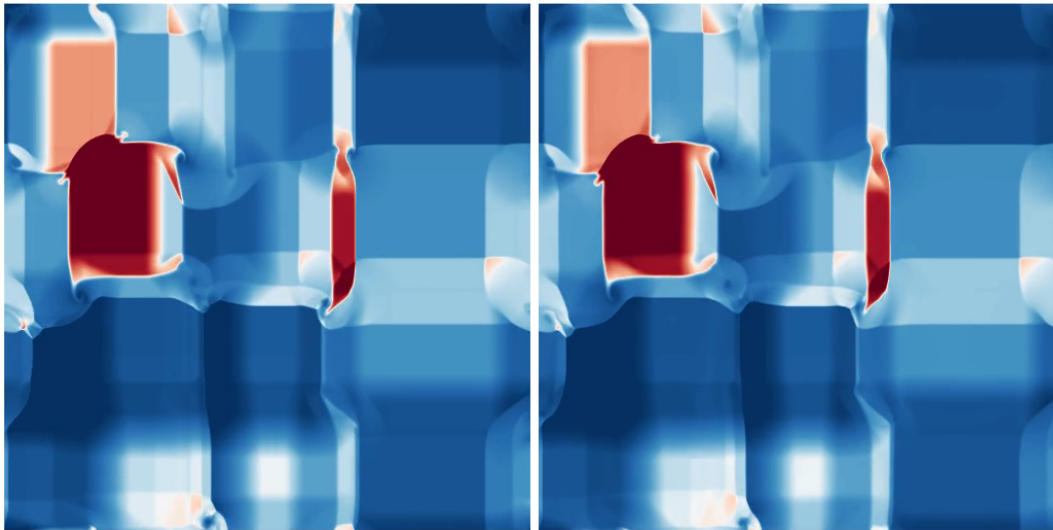


Latent diffusion models for physics emulation

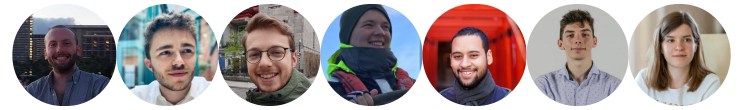


ground-truth

emulated



LDMs trained on compressed latent states $z = E(x)$ remain accurate even at high compression rates.

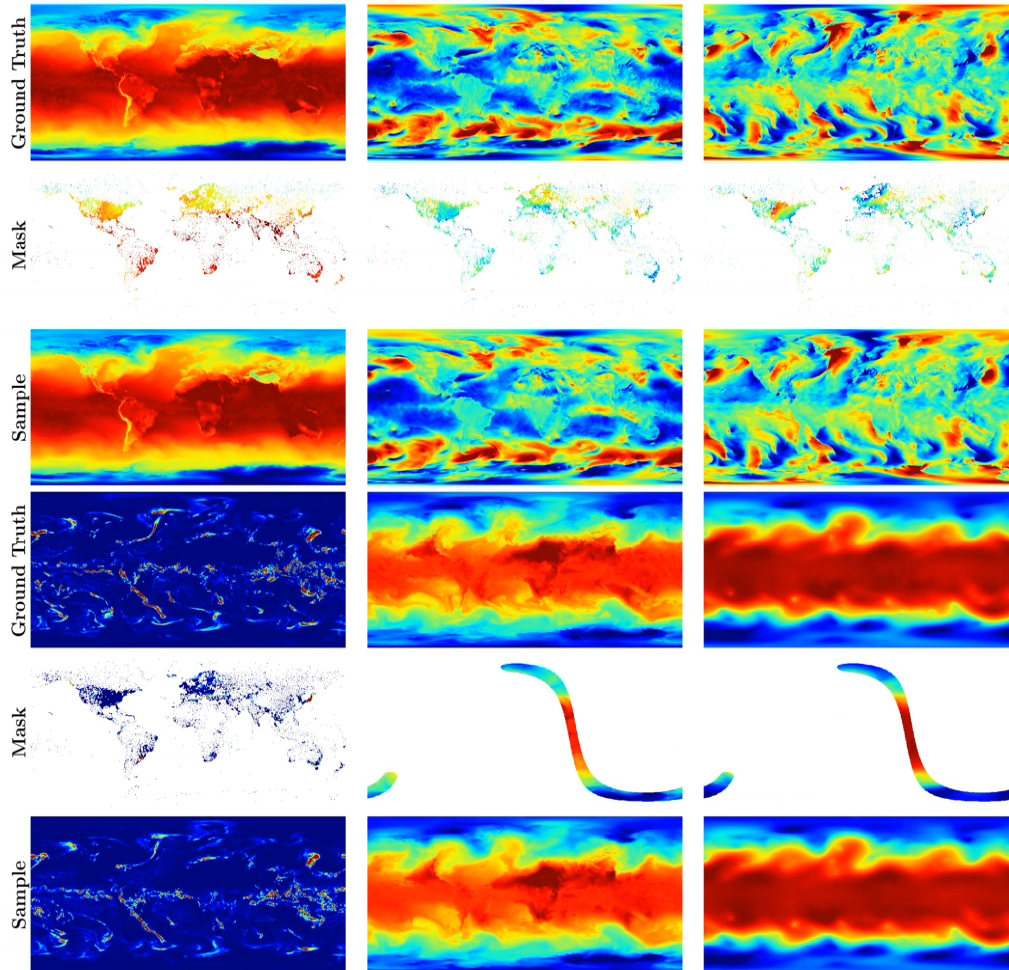


Appa: Bending weather dynamics with LDMs

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 **latent diffusion model** that generates latent trajectories $z_{1:L}$;
- a **posterior sampling algorithm** adapted from MMPS (Rozet et al, 2024) that samples from the posterior distribution $p(z_{1:L} | y)$.

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

Live demo of Appa.



Conclusions

Deep generative models unlock high-dimensional Bayesian inference in complex physical models: **new scientific questions become accessible.**

Next challenges:

- Rigorous validation: when and why these methods work (or not).
- Resolution (in space and time): can we go higher?
- Misspecification: what if the prior, the physical, or the observation models are wrong?



(G rome, Franois, Victor, Omer, Sacha, Matthias, Elise, Malavika, Thomas)

