

Harnessing Low-dimensionality in Diffusion Models

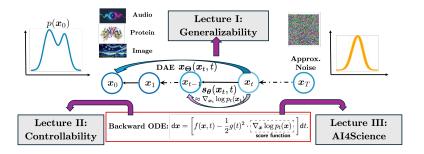
Lecture III: Solving Inverse Problems & AI for Science

Qing Qu

September 22, 2025

EECS, University of Michigan

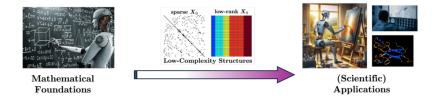
Lecture Schedule



We focus on the **mathematical foundations** of diffusion models through **low-dim structures** and their scientific applications:

- Introduction of Diffusion Models
- Lecture I: Generalization of Learning Diffusion Models
- · Lecture II: Controllability of Diffusion Models
- Lecture III: From Theory to Scientific Applications

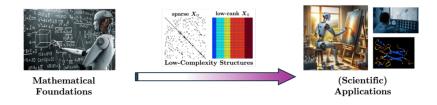
Application of Diffusion Models: Solving Inverse Problems



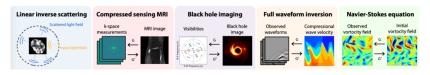
- Inverse problems are common across scientific applications.¹
- Diffusion models learn strong priors to effectively solve them.

¹Zheng et al., InverseBench: Benchmarking Plug-and-Play Diffusion Models for Inverse Problems in Physical Sciences, ICLR 2025.

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Outline

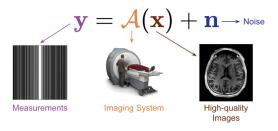
1. Image Reconstruction Problems

2. Data Assimilation

3. Conclusion & Acknowledgement

Image Reconstruction Problems

Inverse Problems



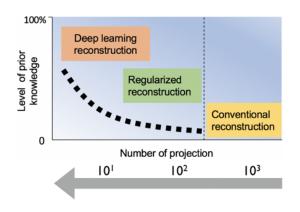
Goal: Recover signal $x \in \mathbb{R}^n$ from noisy measurements $y \in \mathbb{R}^m$ $(m \ll n)$:

$$y = A(x) + n$$

where $\mathcal{A}(\cdot)$ is a forward model, and n is some measurement noise.

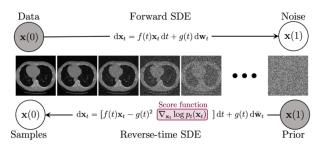
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Leverage Prior Knowledge for Solving Ill-Posed Inverse Problem



- · Conventional method: requires dense sampling
- Regularization method: sparsity in transformed domain
- Data driven method: learned prior from a data-driven way

Recap: Score-based Diffusion Models



- Forward diffusion process as stochastic differential equation (SDE)
- Generative reverse SDE: uses score function to sample from prior $p(\boldsymbol{x})$

Diffusion models learn data prior by modeling **data distribution** through unsupervised training.

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Solving Inverse Problems via Conditional Sampling

Goal: Recover signal $x \in \mathbb{R}^n$ from $y \in \mathbb{R}^m$ ($m \ll n$):

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with forward model $\mathcal{A}(\cdot)$ and noise corruption n.

Solving Inverse Problems via Conditional Sampling

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Idea of applying diffusion models: sampling from p(x|y) instead of p(x) within the diffusion reverse process:

$$abla \log p_t(\boldsymbol{x}_t \mid \boldsymbol{y}) = \underbrace{\nabla \log p_t(\boldsymbol{x}_t)}_{\text{we already have}} + \underbrace{\nabla \log p_t(\boldsymbol{y} \mid \boldsymbol{x}_t)}_{\text{missing \& intractable}}.$$

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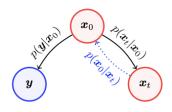
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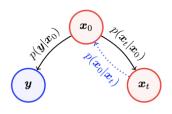
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- Advantages: unsupervised learning with limited assumptions, and comparable or better performance to supervised learning.
- Challenges: Estimating the posterior score $\nabla \log p_t(\boldsymbol{y} \mid \boldsymbol{x}_t)$?



· Posterior score decomposition:

$$\nabla \log p_t(\boldsymbol{x}_t \mid \boldsymbol{y}) = \nabla \log p_t(\boldsymbol{x}_t) + \nabla \log p_t(\boldsymbol{y} \mid \boldsymbol{x}_t)$$



Posterior score decomposition:

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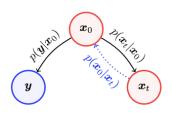
Posterior mean estimation (Tweedie's Formula):

$$\hat{\boldsymbol{x}}_0 := \mathbb{E}[\boldsymbol{x}_0 \mid \boldsymbol{x}_t] = \frac{1}{\sqrt{\bar{\alpha}(t)}} \left(\boldsymbol{x}_t + (1 - \bar{\alpha}(t)) \nabla \log p_t(\boldsymbol{x}_t) \right)$$

• Approximating $abla \log p_t(oldsymbol{y} \mid oldsymbol{x}_t)$ via

$$p(\boldsymbol{y} \mid \boldsymbol{x}_t) \simeq p(\boldsymbol{y} \mid \hat{\boldsymbol{x}}_0).$$

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· Decomposing posterior score:

$$\nabla \log p_t(\boldsymbol{x}_t \mid \boldsymbol{y}) = \nabla \log p_t(\boldsymbol{x}_t) + \nabla \log p_t(\boldsymbol{y} \mid \boldsymbol{x}_t)$$

Take backpropagation through the network:

$$\nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{y} \mid \boldsymbol{x}_t) \simeq \nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{y} \mid \hat{\boldsymbol{x}}_0)$$
$$\simeq -\eta \nabla_{\boldsymbol{x}_t} \|\boldsymbol{y} - \mathcal{A}(\hat{\boldsymbol{x}}_0(\boldsymbol{x}_t))\|_2^2.$$

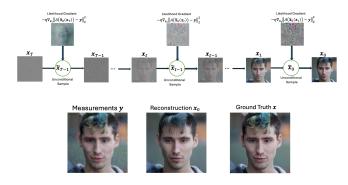


Figure 1: Diffusion Posterior Sampling Process

Guide the unconditional diffusion sampling process with the conditional gradient $-\eta \nabla_{x_t} \|y - \mathcal{A}(\hat{x}_0(x_t))\|_2^2$.

Limitations of Coupled Sampling & Data Consistency

Measurements y





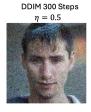


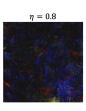


- Limitation 1: large number of sampling steps.
 - To ensure data consistency, it cannot benefit from faster samplers such as DDIM (Song et al. 2020) and Consistency Models (Song et al. 2023).
 - This is because **coupled** sampling and data consistency.

Limitations of DPS







- Limitation 1: large number of sampling steps.
 - Increasing step size η of the likelihood gradient $-\eta \nabla_{x_t} \| \boldsymbol{y} \mathcal{A}(\hat{\boldsymbol{x}}_0(\boldsymbol{x}_t)) \|_2^2$ does not help.
 - The likelihood gradient is also expensive to compute due to backpropagation.

Limitations of DPS



• Limitation 2: Inconsistent reconstructions.

Limitations of DPS



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- Limitation 3: Difficult to adapt to latent diffusion.

Consider the regularized optimization formulation:

$$\min_{\boldsymbol{x}} \frac{1}{2} ||\mathcal{A}(\boldsymbol{x}) - \boldsymbol{y}||_2^2 + \lambda \mathcal{R}(\boldsymbol{x})$$

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Question: How do we **better** utilize the diffusion model as the data prior?

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Question: How do we **better** utilize the diffusion model as the data prior?

• Introducing an auxiliary variable v:

$$\min_{\boldsymbol{x},\boldsymbol{v}} \frac{1}{2} ||\mathcal{A}(\boldsymbol{x}) - \boldsymbol{y}||_2^2 + \lambda \mathcal{R}(\boldsymbol{v}), \text{ s.t. } \boldsymbol{x} = \boldsymbol{v}$$

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· Applying half quadratic splitting (HQS):

$$\min_{x,v} \frac{1}{2} ||\mathcal{A}(x) - y||_2^2 + \mu ||x - v||_2^2 + \lambda \mathcal{R}(v)$$

Alternating minimization between \boldsymbol{x} and \boldsymbol{v} for solving

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· Data consistency optimization via gradient descent:

$$x_k = \underset{x}{\operatorname{arg\,min}} \frac{1}{2} ||\mathcal{A}(x) - y||_2^2 + \mu ||x - v_{k-1}||_2^2$$

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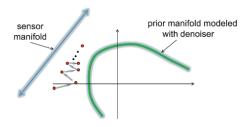
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Enforcing image prior (through diffusion models):

$$v_k = \underset{v_k}{\operatorname{arg\,min}} \mu ||x_k - v||_2^2 + \lambda \mathcal{R}(v)$$



Decoupling via variable splitting and alternating minimization:

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Enforcing image prior (through diffusion models):

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Step I: Data Consistency Optimization



 Data fidelity optimization. Generate measurement-consistent reconstructions (suffer from artifacts):

$$x_k = \underset{x}{\operatorname{arg \, min}} \frac{1}{2} ||\mathcal{A}(x) - y||_2^2 + \mu ||x - v_{k-1}||_2^2,$$

which can be solved via gradient descent.

Step II: Enforcing Image Prior via Diffusion Purification



Question: Can we refine x_k with pre-trained diffusion models?

²Nie et al. Diffusion Models for Adversarial Purification, 2022.

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Question: Can we refine x_k with pre-trained diffusion models?

Solution: Diffusion purification² by adding noise and then denoising

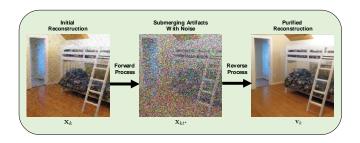
• Run forward process to a certain intermediate noise level t^* .

$$\boldsymbol{x}_{k,t^*} = \boldsymbol{x}_k + \sigma_{t^*} \boldsymbol{\epsilon},$$

• Run the reverse sampling process from x_{k,t^\star} to obtain v_k .

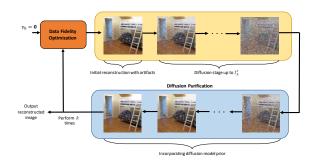
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Step II: Enforcing Image Prior via Diffusion Purification



- Effectiveness: With a properly chosen t*, the image artifacts can be effectively removed while the overall image structures are preserved.
- Efficiency: Diffusion purification can be efficiently implemented through fast samplers, such as DDIM and consistency models. It can also be easily adapted to the latent space.

Decoupled Data Consistency via Diffusion Purification (DCDP)



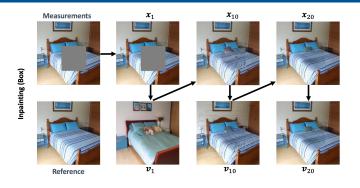
Step I: Enforcing data consistency:

$$m{x}_k = rg \min_{m{x}} rac{1}{2} || \mathcal{A}(m{x}) - m{y} ||_2^2 + \mu || m{x} - m{v}_{k-1} ||_2^2$$

• Step II: Applying diffusion purification:

$$\boldsymbol{v}_k = \mathsf{DPUR}(\boldsymbol{x}_k, t_k^*)$$

Decoupled Data Consistency via Diffusion Purification (DCDP)



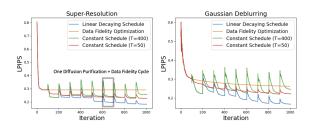
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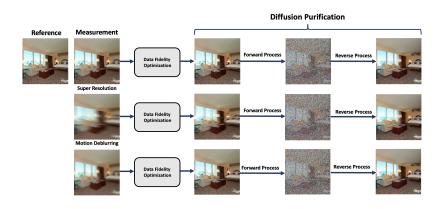
$$x_k = \underset{x}{\operatorname{arg\,min}} \frac{1}{2} ||\mathcal{A}(x) - y||_2^2 + \mu ||x - v_{k-1}||_2^2$$

Applying diffusion purification:

$$\boldsymbol{v}_k = \mathsf{DPUR}(\boldsymbol{x}_k, t_k^*)$$

Use a **decaying** purification strength t_k^{\star} across iteration k for stable convergence.

Effectiveness of Diffusion Purification



• **Effectiveness:** Diffusion Purification is effective for various inverse problems.

Efficiency of Diffusion Purification via DDIM



Figure 2: DPS: insufficient sampling Steps leads to inconsistent samples

Efficiency of Diffusion Purification via DDIM



Figure 2: DPS: insufficient sampling Steps leads to inconsistent samples



Figure 3: DCDP: Fast diffusion purification via DDIM.

Efficiency of Diffusion Purification via Consistency Models



 Diffusion Purification can efficiently be performed using Consistency Models (one step).

Improved Data Consistency via DCDP



• DCDP is more data consistent with the measurements.

Competitive Performance in the Latent Space



Competitive Performance: Quantitative Comparison

Method	Gaussian Deblurring			Motion Deblurring		
Method	LPIPS↓	PSNR↑	SSIM↑	LPIPS↓	PSNR↑	SSIM↑
DPS [14]	0.213 ± 0.08	24.45 ± 3.72	0.691 ± 0.132	0.182 ± 0.03	24.45 ± 2.93	0.736 ± 0.06
MCG [11]	0.311 ± 0.13	17.54 ± 5.06	0.551 ± 0.191	0.365 ± 0.11	20.17 ± 3.73	0.515 ± 0.36
ADMM-PnP [49]	0.437 ± 0.04	20.76 ± 1.94	0.595 ± 0.09	0.524 ± 0.04	18.05 ± 2.05	0.493 ± 0.10
DDNM [13]	0.217 ± 0.07	27.30 ± 1.67	0.815 ± 0.08	-	-	-
RED-Diff [45]	0.228 ± 0.12	23.98 ± 1.23	0.687 ± 0.067	0.178 ± 0.06	24.15 ± 2.34	0.704 ± 0.12
DiffPIR [50]	0.214 ± 0.013	27.04 ± 2.67	0.801 ± 0.12	0.114 ± 0.12	27.45 ± 1.89	0.866 ± 0.65
DCDP-DDIM (Ours)	0.196 ± 0.05	27.13 ± 3.26	0.804 ± 0.07	0.065 ± 0.01	33.56 ± 3.92	0.947 ± 0.02
DCDP-Tweedie (Ours)	0.212 ± 0.05	27.74 ± 3.34	0.825 ± 0.07	0.067 ± 0.02	34.47 ± 4.07	0.956 ± 0.02
Latent-DPS	0.337 ± 0.05	23.75 ± 2.53	0.622 ± 0.10	0.425 ± 0.06	21.90 ± 2.31	0.539 ± 0.10
PSLD [18]	0.373 ± 0.07	24.26 ± 2.84	0.683 ± 0.11	0.469 ± 0.06	20.58 ± 2.32	0.562 ± 0.11
ReSample [19]	0.240 ± 0.05	25.76 ± 3.02	0.731 ± 0.09	0.188 ± 0.04	27.96 ± 3.07	0.806 ± 0.07
DCDP-LDM-DDIM (Ours)	0.246 ± 0.05	26.08 ± 3.02	0.766 ± 0.07	0.145 ± 0.03	28.87 ± 3.77	0.856 ± 0.06
DCDP-LDM-Tweedie (Ours)	0.217 ± 0.05	27.11 ± 3.26	0.807 ± 0.07	0.121 ± 0.03	29.40 ± 3.81	0.875 ± 0.05
DCDP-CMs (Ours)	0.202 ± 0.05	26.91 ± 3.11	0.805 ± 0.07	0.061 ± 0.02	34.10 ± 3.80	0.953 ± 0.02

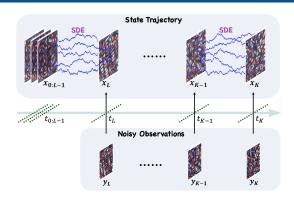
Discussion

- Diffusion models can serve as an implicit regularization for solving ill-posed inverse problems.
- Decoupling the data consistency can significantly improve the efficiency and flexibility.
- Limitation: Perception-distortion tradeoff (a potential direction to explore)

 Xiang Li, Soo Min Kwon, Ismail R. Alkhouri, Saiprasad Ravishankar, Qing Qu. Decoupled Data Consistency with Diffusion Purification for Image Restoration. Under Review at IEEE Journal of Selected Topics in Signal Processing (JSTSP), 2025.

Data Assimilation

Background: Data Assimilation



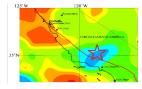
Stochastic dynamic systems:

$$oldsymbol{x}_k = egin{array}{c} \Psi(oldsymbol{x}_{k-1}) &+ oldsymbol{\xi}_{k-1} \ ext{transition map} & ext{stochastic force} \end{array}$$

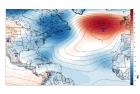
• (Partial) nosiy observation models:

$$oldsymbol{y}_k = egin{array}{c} \mathcal{A}(oldsymbol{x}_k) &+ oldsymbol{\eta}_k \ ext{partial observation} \end{array}$$

Background: Data Assimilation







Earthquake Prediction

Weather Forecasting

Hurricane Prediction

Data Assimilation (DA): combine observations y_k with numerical models to **predict states** x_k in stochastic dynamic systems.

$$egin{array}{lll} x_k &=& \Psi(x_{k-1}) \; + \; & oldsymbol{\xi}_{k-1} \ & & ext{transition map} \end{array},$$

$$oldsymbol{y}_k = egin{array}{c} \mathcal{A}(oldsymbol{x}_k) & + oldsymbol{\eta}_k. \ & ext{partial observation} \end{array}$$

Classical Approaches for DA

Model-based methods (require state transition model Ψ):

 Kalman filter: assumption of Gaussian noise and linear dynamics

$$egin{aligned} x_k &= A x_{k-1} + B u_{k-1} + w_{k-1} \ \hat{x}_{k|k} &= \hat{x}_{k|k-1} + K_k \left(z_k - H \hat{x}_{k|k-1}
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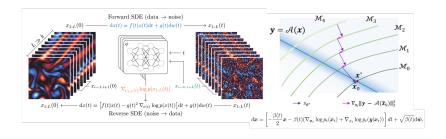
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 Particle filter: curse of dimensionality, computationally too expensive in high-dimension

$$egin{aligned} oldsymbol{x}_k^i &= \Psi(oldsymbol{x}_{(k-1)}^i) + oldsymbol{\xi}_k^i \ \hat{oldsymbol{x}}_k &= \sum_{i=1}^N \omega_k^i oldsymbol{x}_k^i, \quad \omega_k^i \propto p(oldsymbol{y}_k \mid oldsymbol{x}_k^i) \end{aligned}$$

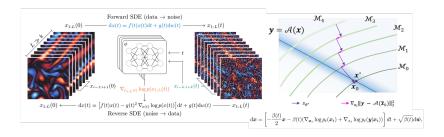
Data-driven Methods for DA



Data-driven methods:

• Score-based diffusion models (SDA): learn joint distribution $p(x_{k-\tau}, \cdots, x_k, \cdots, x_{k+\tau} \mid y_{k+\tau})$ of state priors (non-autoregressive)

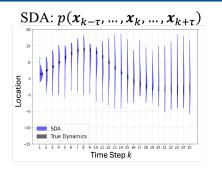
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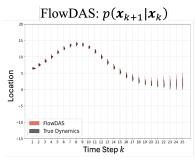


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- Our Method: FlowDAS explicitly models system transition dynamics $p(x_k \mid x_{k-1}, y_k)$ (autoregressive)

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• Learning a predictor: estimate $x_k' \sim \pi_{\theta}(x_k' \mid x_{k-1})$ via stochastic interpolant (SI).³

 $^{^3}$ M. S. Albergo et al., Stochastic Interpolants: A Unifying Framework for Flows and Diffusions.

⁴H. Chung et al., Diffusion Posterior Sampling for General Noisy Inverse Problems

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- Correction using partial observation: leverage y_k to estimate $q(x_k \mid x_k', y_k)$ inspired by denoising posterior sampling (DPS)⁴.

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- Learning a predictor: estimate $x_k' \sim \pi_{\theta}(x_k' \mid x_{k-1})$ via stochastic interpolant (SI).³
- Correction using partial observation: leverage y_k to estimate $q(x_k \mid x_k', y_k)$ inspired by denoising posterior sampling (DPS)⁴.
- Autoregressive: estimate $m{x}_{k+1} \sim q(m{x}_{k+1} \mid m{x}_k, m{y}_{k+1})$ and repeat.

 $^{^3}$ M. S. Albergo et al., Stochastic Interpolants: A Unifying Framework for Flows and Diffusions.

⁴H. Chung et al., Diffusion Posterior Sampling for General Noisy Inverse Problems

Stochastic Interpolants (SI) for Probabilistic Forecasting

Consider a stochastic process X_s defined over the interval $s \in [0,1]$, evolving from initial state X_0 to X_1 . The SI can be described as

$$\boldsymbol{X}_s = \alpha_s \boldsymbol{X}_0 + \beta_s \boldsymbol{X}_1 + \sigma_s \boldsymbol{W}_s$$

where $\alpha_s, \beta_s, \sigma_s$ are drift coefficients, and W_s is a Wiener process.

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• Let $b_s(X_s,X_0)$ be the "velocity" of the interpolant path, then X_s follows the SDE

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• The drift (velocity) term $oldsymbol{b}_s(oldsymbol{X}_s,oldsymbol{X}_0)$ can be learned through

$$\mathcal{L}_b(\hat{\boldsymbol{b}}_s) = \int_0^1 \mathbb{E}\left[\|\hat{\boldsymbol{b}}_s(\boldsymbol{X}_s, \boldsymbol{X}_0) - \boldsymbol{R}_s\|^2\right] ds.$$

where $\mathbf{R}_s = \dot{\alpha}_s \mathbf{X}_0 + \dot{\beta}_s \mathbf{X}_1 + \dot{\sigma}_s \mathbf{W}_s$.

Observation Consistent Prediction

To ensure measurement consistency $m{y}=\mathcal{A}(m{x})$, FlowDAS augments the original drift $m{b}_s(m{X}_s,m{X}_0)$ via Bayes' rule

$$\boldsymbol{b}_s(\boldsymbol{X}_s, \boldsymbol{y}, \boldsymbol{X}_0) = \boldsymbol{b}_s(\boldsymbol{X}_s, \boldsymbol{X}_0) + \frac{\nabla \log p(\boldsymbol{y} \mid \boldsymbol{X}_s, \boldsymbol{X}_0)}{\lambda_s \beta_s}.$$

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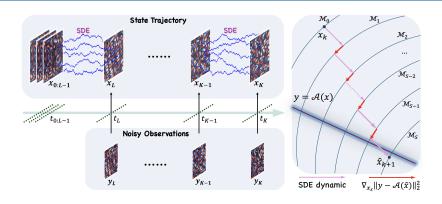
- The conditional score $\nabla \log p(y \mid X_s, X_0)$ captures the observation information, but intractable.
- In practice, we estimate it by Monte-Carlo marginalization and do Monte Carlo sampling during inference.

Algorithm 2 Inference

```
1: Input: Observation y_{L:K}, the measurement map \mathcal{A}, initial state x_0, model \hat{b}_s(X, X_0), noise
      coefficient \sigma_{s_{\ell}} grid s_0 = 0 < s_1 < \cdots < s_N = 1, i.i.d. \boldsymbol{z}_n \sim \mathcal{N}(0, \boldsymbol{I}_D) for n = 0 : N - 1, step size
      \zeta_n, Monte Carlo sampling times J

 Set x̂<sub>L-1</sub> ← x<sub>L-1</sub>

 3: Set the (\Delta s)_n = s_{n+1} - s_n, \ n = 0: N-1
 4. for k = L - 1 to K - 1 do
         X_{so}, y \leftarrow \hat{x}_{b}, y_{b+1}
         for n = 0 to N - 1 do
              X'_{s_{n+1}} = X_{s_n} + \hat{b}_s(X_{s_n}, X_{s_0})(\Delta s)_n + \sigma_{s_n} \sqrt{(\Delta s)_n} z_n
 7.
              \{\hat{\boldsymbol{X}}_{1}^{(j)}\}_{i=1}^{J} \leftarrow \text{Posterior estimation } (\hat{\boldsymbol{b}}_{s}, s_{n}, \boldsymbol{X}_{0}, \boldsymbol{X}_{s_{n}})
              \{w_j\}_{j=1}^J \leftarrow \operatorname{Softmax}\left(\{\|\boldsymbol{y} - \mathcal{A}(\hat{\boldsymbol{X}}_1^{(j)})\|_2^2\}_{j=1}^J\right)
              X_{s_{n+1}} = X'_{s_{n+1}} - \zeta_n \nabla_{X_{s_n}} \sum_{j=1}^{J} w_j \| y - \mathcal{A}(\hat{X}_1^{(j)}) \|_2^2
10:
          end for
11.
          \hat{\boldsymbol{x}}_{k+1} \leftarrow \boldsymbol{X}_{s_N}
12:
13: end for
14: return \{\hat{\boldsymbol{x}}_k\}_{k=L}^K
```



- Physics aligned transport: directly learns transition between adjacent states, enabling faster inference and stable training
- Observation-consistency: learns the full conditional distribution, with no post-hoc update needed

Low-dimensional Problem: Lorenz 1963

- Stuyd the 3D Lorenz 1963 tracking problem, with $x(t) = (x_1(t), x_2(t), x_3(t))$.
- · System dynamics:

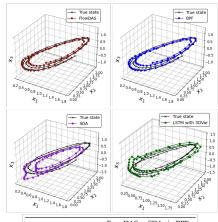
$$\frac{dx_1}{dt} = \mu(x_2 - x_1) + \xi_1$$

$$\frac{dx_2}{dt} = x_1(\rho - x_3) - x_2 + \xi_2$$

$$\frac{dx_3}{dt} = x_1x_2 - \tau x_3 + \xi_3$$

· Observation model:

$$y = \arctan(x_1) + \eta$$



		FLOWDAS	SDA	BPF
\uparrow	$\log p(\hat{x}_{2:K} \hat{x}_1)$	17.29	-332.7	17.88
1	$\log p(\boldsymbol{y} \mid \hat{\boldsymbol{x}}_{1:K})$	-0.228	-6.112	-1.572
1	$W_1(x_{1:K}, \hat{x}_{1:K})$	0.106	0.528	0.812
1	$RMSE(\boldsymbol{x}_{1:K}, \hat{\boldsymbol{x}}_{1:K})$	0.202	1.114	0.270

Solving Navier-Stokes (NS) Equation

- Consider the **incompressible fiuld flow** governed by 2D NS equations. Let $x=\omega$ to be the *vorticity field*.
- State transition dynamics:

$$d\omega + \mathbf{v} \cdot \nabla \omega \, dt = \nu \Delta \omega \, dt - \alpha \omega \, dt + \epsilon \, d\xi.$$

• Observation model: $y = A(\omega) + \eta$, where A could be downsampling operator or random mask.

Solving Navier-Stokes (NS) Equation

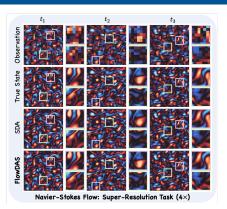
	$32^2 \rightarrow 128^2$	$16^2 \rightarrow 128^2$	5%	1.5625%
FLOWDAS	0.038	0.067	0.071	0.123
FNO-DA	0.158	0.166	0.165	0.183
TRANSOLVER-DA	0.159	0.176	0.161	0.180
SDA	0.073	0.133	0.251	0.258

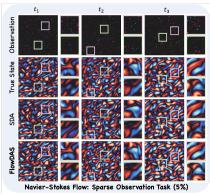
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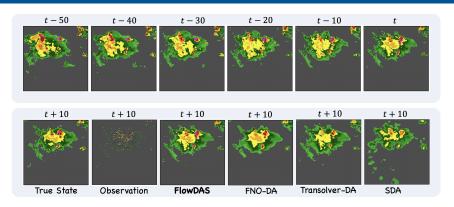
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Application I: Weather Forecasting on SEVIR Dataset

- Storm Event ImageRy (SEVIR) is a spatiotemporal Earth observation dataset which consists of $384~\rm km \times 384~\rm km$ image sequences spanning over 4 hours.
- Task: predict the future Vertically Integrated Liquid (VIL) given of pervious context VIL and some sparse observation (10%)

Application I: Weather Forecasting on SEVIR Dataset



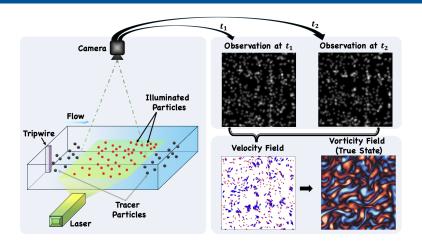
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Application I: Weather Forecasting on SEVIR Dataset

METHOD	RMSE ↓	CSI($ au_{20}$) (0.3) \uparrow	CSI($ au_{40}$) (0.5) \uparrow
TRANSOLVER-DA	0.062±0.001	0.663±0.001	0.499±0.002
FNO-DA	0.064 ± 0.001	0.641 ± 0.001	0.493 ± 0.002
SDA	0.071±0.007	0.549 ± 0.033	0.387 ± 0.065
FLOWDAS	0.053±0.004	0.746 ± 0.022	0.614 \pm 0.044

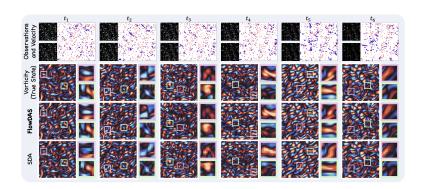
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Application II: Particle Image Velocimetry (PIV)



- For many scientific applications, PIV aims at measuring dense vorticity fields from sparse velocity measurements.
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Discussion

- Method: We introduce FlowDAS, a flow-based autoregressive method for solving the data assimilation problem with many scientific applications.
- Significance: the first DA framework built on stochastic interpolants that learns step-to-step state transitions and conditions on observations during rollout.
- Future directions: multimodality and multiphyics, long-term prediction, efficiency, and robustness.
- Siyi Chen*, Yixuan Jia*, Qing Qu, He Sun, Jeffrey Fessler. FlowDAS: A Stochastic Interpolant-based Framework for Data Assimilation. Neural Information Processing Systems (NeurIPS'25), 2025.

Conclusion & Acknowledgement

Take-Home Message

- Solving image reconstruction problems: We developed an efficient method for solving image inverse problems through decoupling via diffusion purification.
- Data assimilation: We explored stochastic interpolant methods for data assimilation in scientific applications, by better modeling the underlying physics.

Major References

- Xiang Li, Soo Min Kwon, Ismail R. Alkhouri, Saiprasad Ravishankar, Qing Qu. Decoupled Data Consistency with Diffusion Purification for Image Restoration. Under Review at IEEE Journal of Selected Topics in Signal Processing (JSTSP), 2025.
- Siyi Chen*, Yixuan Jia*, Qing Qu, He Sun, Jeffrey Fessler. FlowDAS: A Stochastic Interpolant-based Framework for Data Assimilation. Neural Information Processing Systems (NeurIPS'25), 2025.
- Ismail Alkhouri, Shijun Liang, Cheng-Han Huang, Jimmy Dai, Qing Qu, Saiprasad Ravishankar, Rongrong Wang. SITCOM: Step-wise Triple-Consistent Diffusion Sampling for Inverse Problems. International Conference on Machine Learning (ICML'25), 2025.
- Bowen Song*, Soo Min Kwon*, Zecheng Zhang, Xinyu Hu, Qing Qu, Liyue Shen. Solving Inverse Problems with Latent Diffusion Models via Hard Data Consistency. International Conference on Learning Representations (ICLR'24), 2024. (spotlight, top 5%)

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Thank You!