ConvLEO: Learning Spatial Priors for Plume Dynamics

Single-shot, arbitrary-time query from any observation time (no rollout error accumulation)

Khalid Rafiq[1], Aditya G. Nair[1]

[1]University of Nevada, Reno

Data + Task: Wind-conditioned plume forecasting

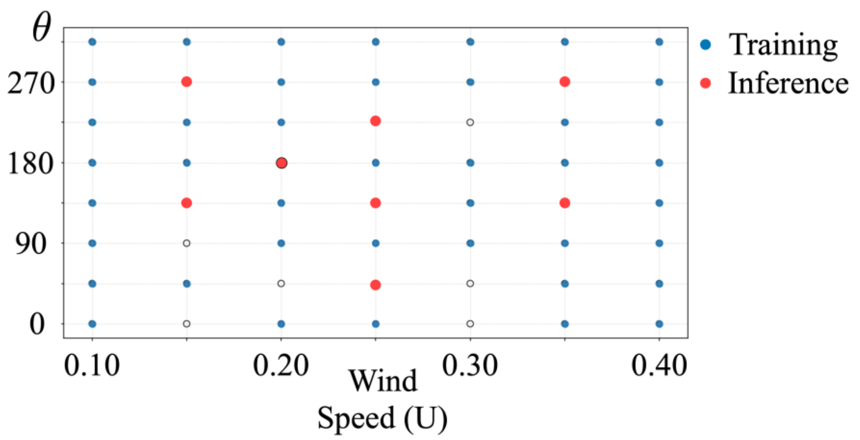
1. The Generative Mechanism[1]

- **Source:** Poisson release of Lagrangian puffs.
- **Dynamics:** advection + radial growth + stochastic perturbations.
- **Frames:** render puffs → $u(x,t) \in \mathbb{R}^{512\times512}$ concentration maps.
- **Number of Frames:** 200 covering 10 seconds of physical time.

One Trajectory $U = 0.25, \theta = 135^\circ$

2. Parametric Dataset Generation

- **Parameter sweep:** A systematic grid sweep over wind speed $(U \in [0.1, 0.4])$ and direction $(\theta \in [0^\circ, 360^\circ])$.
- **Held-out generalization:** red points (unseen (U,θ) combinations).



3. Task (LEO – Latent Evolution Operator)

- Given **one noisy snapshot** $u(x,t)$ and parameters (U,θ) and time jump (τ) predict $u(t+\tau)$.

[1]https://github.com/florisvb/ParallelPlumeSim

Where we fit: Autoregressive vs Operator Learning vs LEO

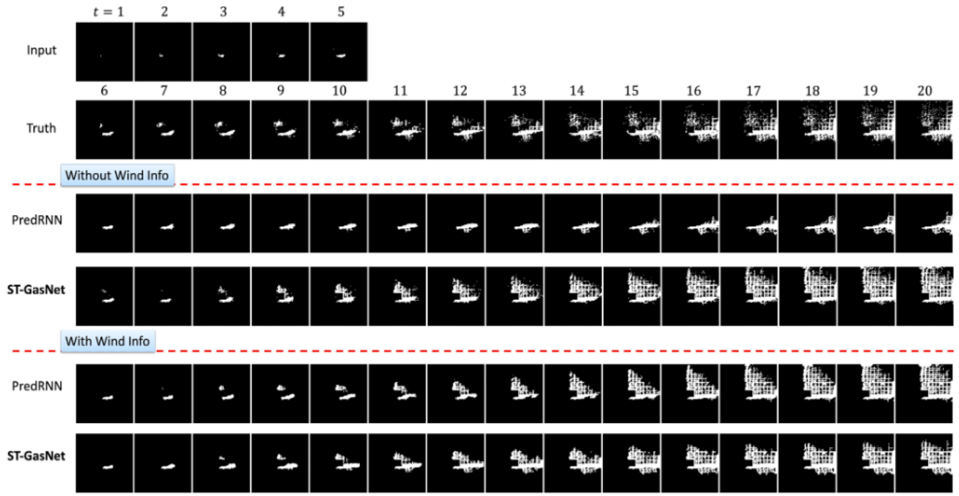
Autoregressive (ConvLSTM / PredRNN / ST-GasNet):
- **Input:** past frames.
- **Output:** next frame(s) step-by-step.
- **Limitation:** *multi-step rollout required; cannot query arbitrary τ from a single snapshot.*

Neural Operators (FNO / DeepONet-style):
- **Input:** typically, initial condition (anchor at t = 0) + query time.
- **Output:** u(t) queried in one-shot.
- **Limitation:** *often assumes a fixed anchor; less natural for "start from any observed time".*

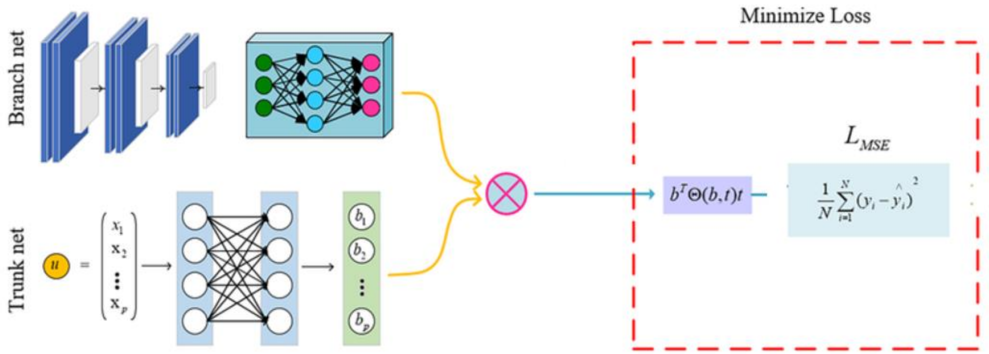
Need: arbitrary-time queries from arbitrary observation times.

Ours (ConvLEO / Latent Evolution Operator[3]):
- **Input: single observation (field)** $+(U,\theta)$ + query(τ) .
- **Output: u(t+τ)** directly via latent flow map.
- **Key benefit: no rollout** — *single-shot u(t+τ) from any observation time.*

ST-GasNet[1]: wind-conditioned spatiotemporal forecasting via autoregressive rollout.



DeepONet[2]: one-shot query u(t) but typically trained around a **fixed anchor** (often t=0)



[1]https://doi.org/10.1093/pnasnexus/pgaf198
[2]https://doi.org/10.1038/s42256-021-00302-5
[3]https://arxiv.org/html/2505.09063v1

Theory & Architecture: The Latent Evolution Operator

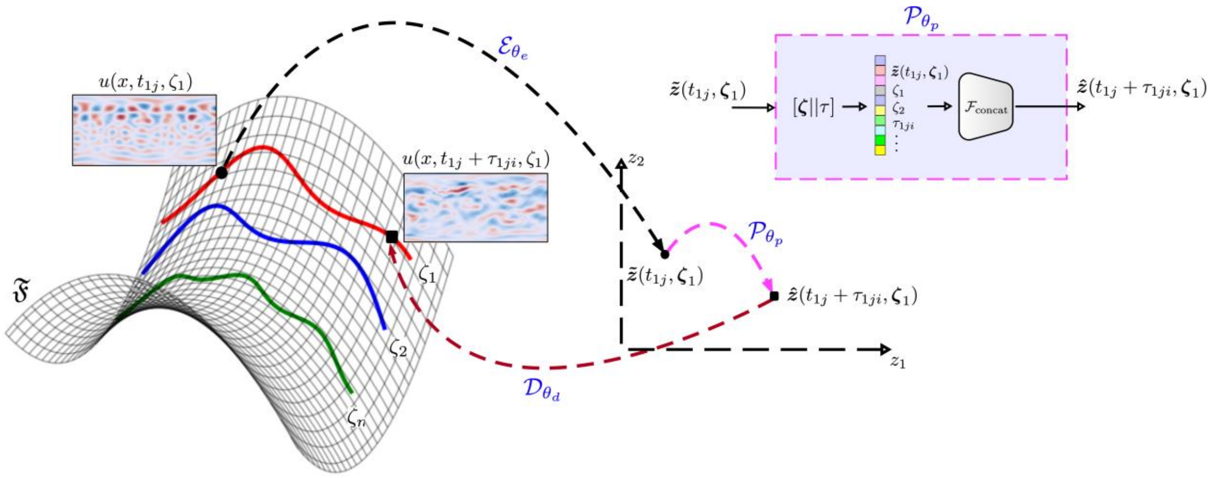
Need: query $u(t_1+\tau)$ from any t_1 using one snapshot, without rollouts.

Key idea:
Learn a *parametric flow map* in latent space.

$$u(t) \xrightarrow{\mathcal{E}} z(t) \xrightarrow{\mathcal{P}(;,\zeta,\tau)} z(t+\tau) \xrightarrow{\mathcal{D}} \hat{u}(t+\tau)$$

Conditioning: $\zeta = [U, \sin(\theta), cos(\theta), \tau]$

LEO Perspective



LEO Skeletal:

Original Latent

$$u(x,t) \xrightarrow{\mathcal{E}_{\theta_e}} z(t) \longrightarrow \oplus \xrightarrow{\mathcal{P}_{\theta_p}(z(t), U, \sin(\theta), \cos(\theta), \tau)} z(t+\tau) \xrightarrow{\mathcal{D}_{\theta_d}} u(x, t+\tau)$$

$$\zeta = [U, \sin(\theta), cos(\theta), \tau] \xrightarrow{\mathcal{P}_{\theta_{\text{proj}}}} \oplus$$

Parameter Informed Latent

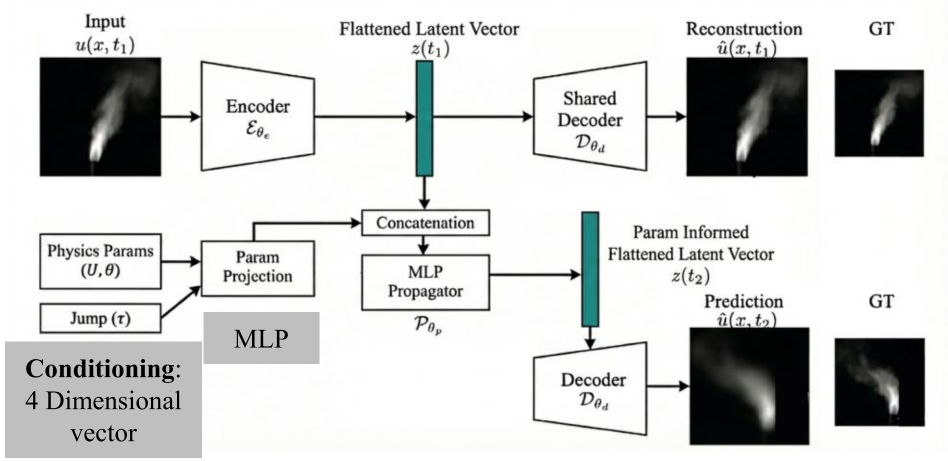
Training Objective:
The model is trained by minimizing a joint loss function that balances current state representation with future state prediction:

$$\mathcal{L} = \|u(t) - \hat{u}(t)\|_2^2 + \lambda_{\text{pred}} \, \|M \odot (u(t+\tau) - \hat{u}(t+\tau))\|_2^2$$

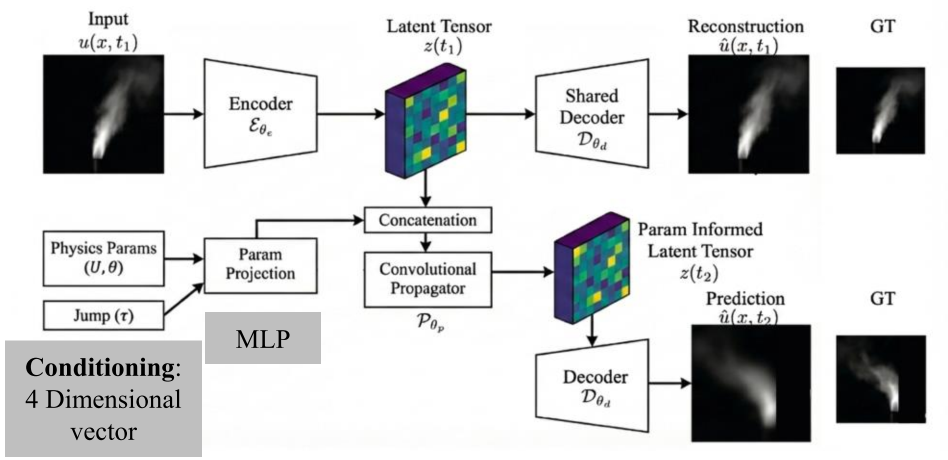
- <u>**Mask-weighted to avoid background dominance (plume is extremely sparse).**</u>

Ablation: Spatial Latents + Physics Injection Prevent Blobbing, (u(t1), U,θ,τ) → u(t2) and NO ROLLOUT

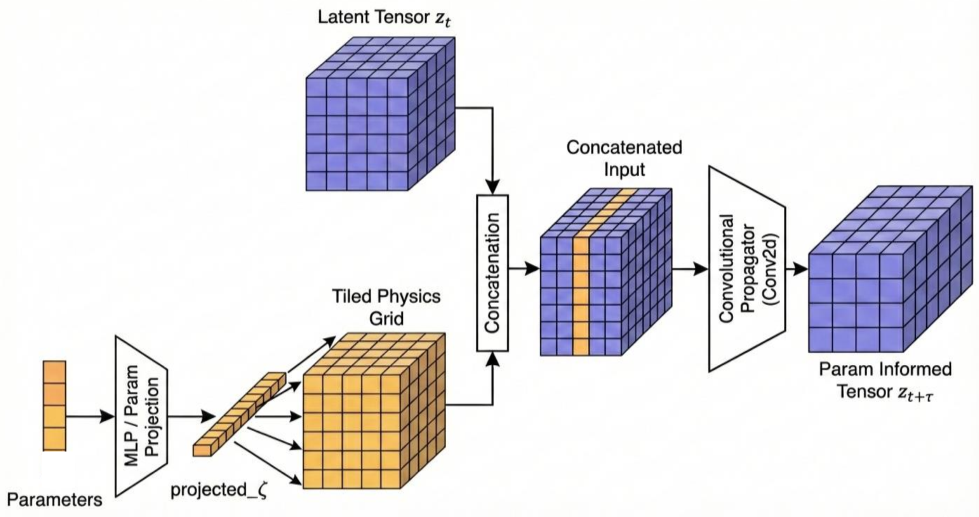
Flattened LEO (vector latent + MLP):
- *Blobbing* → loses spatial topology.



ConvLEO (spatial latent + conv):
- *Tracks advection* due to translation equivariance + local receptive fields.



Heart of ConvLEO: Spatial Physics Injection
- Global parameters ζ are projected into a nonlinear embedding and spatially broadcasted to form a grid. This 'physics-tensor' conditions the convo propagator to steer latent features with precise advection and diffusion.



$$\zeta = [U, \sin(\theta), cos(\theta), \tau]$$

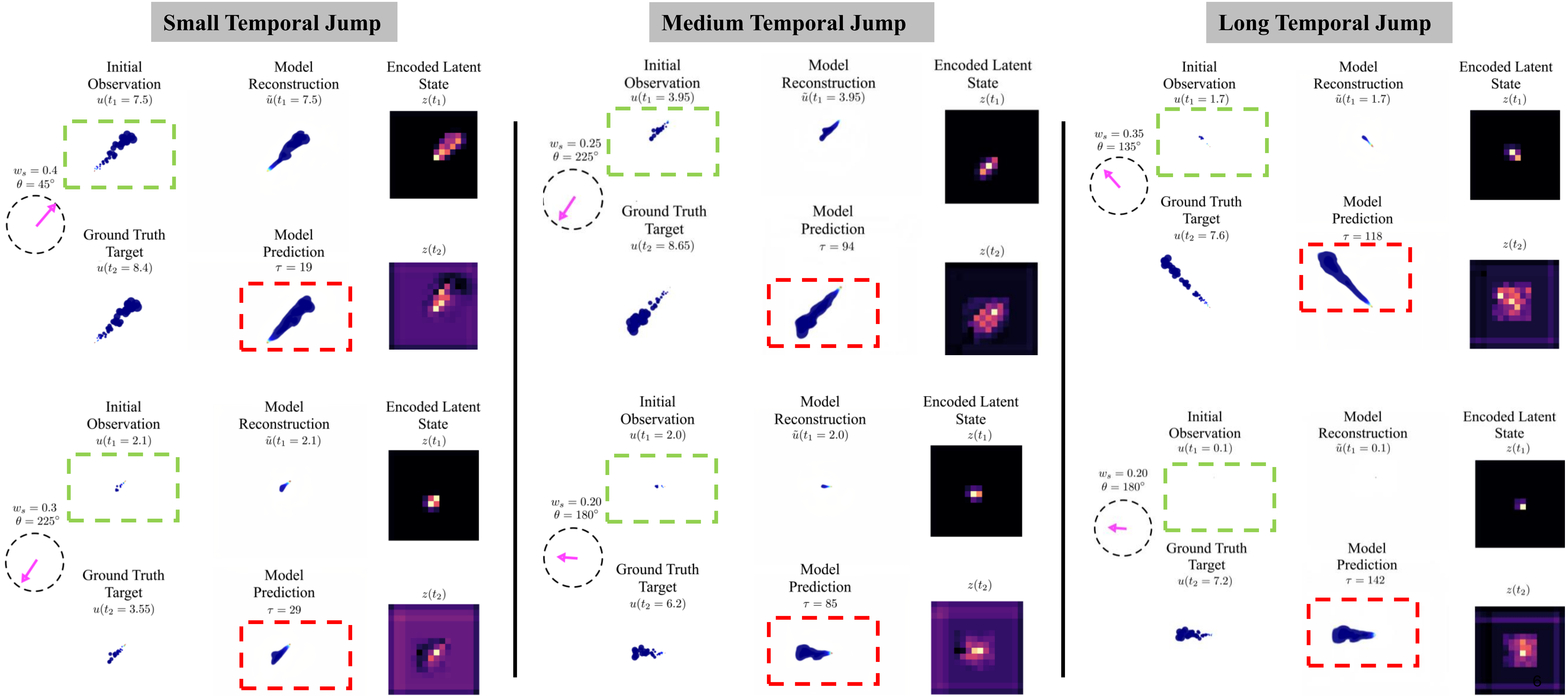
Optimization & Hyperparameter Convergence
- 15-trial BO (W&B) optimizing held-out (U, θ) for generalization and minimizing L_{val} .
- **Best Configuration:**

$$z_c = 256, \zeta_c = 32, \lambda_{mask} = 130, \lambda_{pred} = 1.2$$

Output of a small Hyper-parameter sweep.

ConvLEO forecasts preserve plume transport and morphology

Green box = observed u(t_1); Red box = single-shot prediction $\hat{u}(t_2)$; forecast u(t_2) from one snapshot +(U, θ, τ), NO ROLL-OUTS



Key Initial Takeaways: What Works, What Breaks, and Why

- **Iso-contour height maps are a poor learning target (topology is discontinuous).**
  Components can **appear / disappear / merge / split**, creating non-smooth evolution that breaks operator/LEO learning.

- **ConvLEO > BaseLEO for transport-dominated dynamics.**
  Spatial latents + **translation equivariance** + **local receptive fields** preserve plume advection and morphology better than a flattened latent + MLP.

- **Spatial physics injection is an effective conditioning mechanism.**
  Broadcasting $\zeta=[U, \sin\theta, \cos\theta, \tau]$ into a grid **steers latent transport** and reduces “**blobbed**” predictions.

- **Sparsity-aware training is mandatory (masking prevents background dominance).**
  Without mask-weighted loss, the model optimizes background and collapses to **blobs / washed-out fields**.

- **Single-shot arbitrary-time querying avoids rollout drift.**
  ConvLEO predicts $u(t_1+\tau)$ directly from one snapshot at any t_1, preventing **error accumulation** common in autoregressive rollouts and avoids running the simulator for context length snapshots.

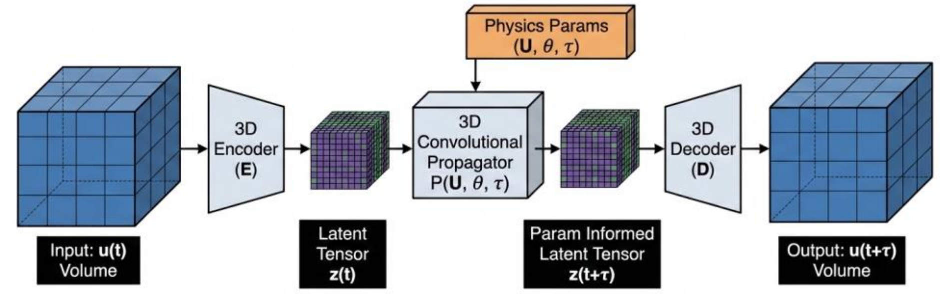
Future Directions – 4D Prediction, Partial Sensing and Inverse Mapping

3D ConvLEO: Volumetric plume forecasting
- **Goal:** 2D frames → 3D volume $u(x, y, z, t)$ conditioned on (U, θ).
- **Method:** swap 2D conv blocks for **3D** Enc/Prop/Dec while keeping the **ConvLEO** framework.
- **Impact:** *single-shot 3D nowcasting at arbitrary t+τ* ***without rollout***

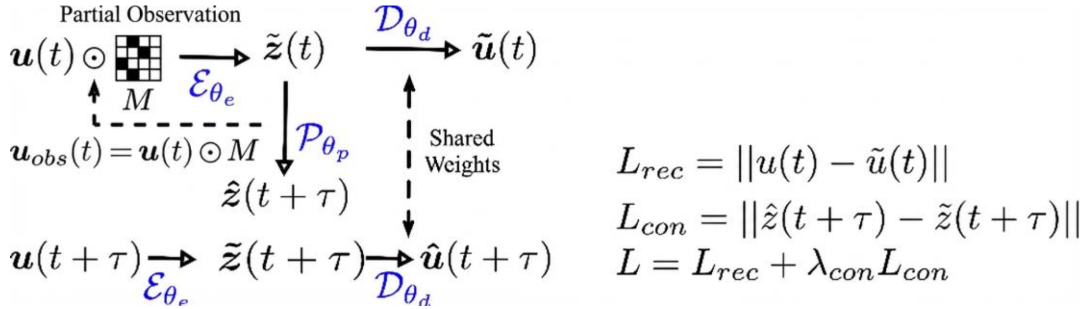
Consistent ConvLEO: Single-shot from sparse observations
- **Goal:** full-field dynamics from **partial observations** $u_{\text{obs}}(t) = M \odot u(t)$.
- **Method: dual encoders** + **latent alignment** so partial-latent ≈ full-latent, alongside recon/pred losses.
- **Impact:** *bridges to real sparse sensor networks*

Bidirectional / Inverse ConvLEO: Effect → Cause
- **Goal:** allow **general time queries** using (t_1, t_2) , not just τ.
- **Method:** learn **time-directional propagation** in latent space for forward direction $t_1 < t_2$ and backward $t_2 < t_1$.
- **Impact:** *source localization + data assimilation*

3D ConvLEO: Volumetric Plume Forecasting



Consistent ConvLEO: Extension to partial observations



Bidirectional ConvLEO: Effect → Cause