Data-Driven Weather Prediction

A Probabilistic Forecasting Framework

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NVIDIA Research

Probabilistic Weather Forecasting

Weather Forecasting

- Immediate impact to disaster preparedness and global markets.
- Guide design and application of climate models.

Probabilistic Modeling

- The atmosphere is chaotic and initial conditions are uncertain.
- Deterministic forecasts are impractical for risk management.

Data-Driven Models

- Massive historical datasets.
- Advances in neural architectures and generative modeling.
- Orders-of-magnitude faster inference than traditional solvers.
- Large ensembles enable real-time probabilistic forecasting.

Problem Formulation

Atmospheric State Representation

Consider a stationary, Markovian, discrete-time stochastic process

$$\{x_j\}_{j\in\mathbb{Z}} \subset \mathbb{R}^d; \qquad p(x_j, x_{j+1}) = p(x_k, x_{k+1}),$$

representing atmospheric states.

Learning Objective

Estimate conditional transition density

$$p(x_1 \mid x_0)$$

from identically distributed samples $(x_j^\dagger, x_{j+1}^\dagger) \sim p(x_0, x_1)$.

Forecast Generation

Autoregressive rollout:

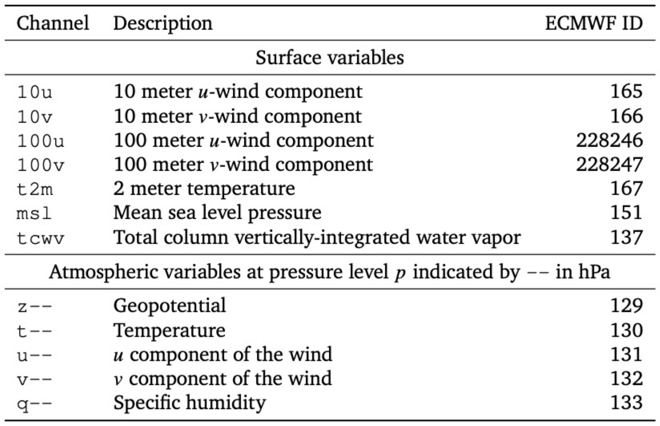
$$\hat{x}_{k+1} \sim p(\cdot \mid \hat{x}_k).$$

Challenges:

(1) high dimensionality $d \gg 1$; (2) distribution shift in rollout.

ERA5 Dataset 1980-2020

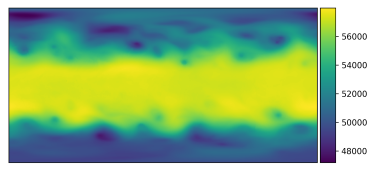
ERA5 Reanalysis Data



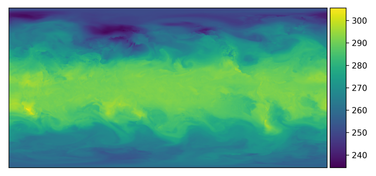
Channel	Description	ECMWF ID
	Surface variables	
`10u`	10 meter *u*-wind component	165
`10v`	10 meter *v*-wind component	166
`100u`	100 meter *u*-wind component	228246
`100v`	100 meter *v*-wind component	228247
`t2m`	2 meter temperature	167
`msl`	Mean sea level pressure	151
`tcwv`	Total column vertically-integrated water vapor	137
	Atmospheric variables at pressure level *p* indicated by `--` in hPa	
`z--`	Geopotential	129
`t--`	Temperature	130
`u--`	*u* component of the wind	131
`v--`	*v* component of the wind	132
`q--`	Specific humidity	133

- Grid: 721 × 1440 equiangular (0.25 deg).
- Sampling interval: 6 hours.
- Structure: 5 atmospheric (13 vertical level) and 7 surface variables.

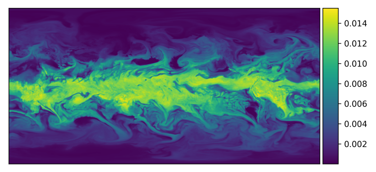
ERA5 Dataset Examples



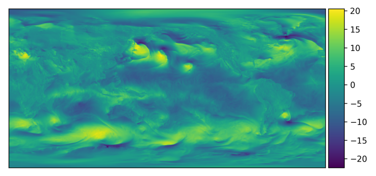
Geopotential (m^2s^{-2}) at 500 hPa



Temperature (K) at 850 hPa



Specific humidity ($kgkg^{-1}$) at 850 hPa



Longitudinal component of wind velocity (ms^{-1}) at 10 m

Properties of Atmospheric Data

Predictability and Length Scales

Atmospheric predictability is scale-dependent:

$$\tau(k) \sim \lambda(k)^{-1},$$

where $\lambda(k)$ is the Lyapunov exponent at wavenumber k.

- Synoptic scales ($\gtrsim$ 1000 km): $\tau \sim$ days.
- Mesoscales ($\lesssim$ 100 km): $\tau \sim$ hours.

At 6 hours, scales below $\approx$ 50–100 km are effectively unpredictable.

Energy Spectrum Considerations

Observed atmospheric kinetic energy spectrum:

$$E(k) \sim \begin{cases} k^{-3} & \text{(synoptic range)} \\ k^{-5/3} & \text{(mesoscale range)} \end{cases}$$

Most forecast-relevant variance lies at low k.

Latent Space Modeling

Latent Representation

Define downsampling operator $B : \mathbb{R}^d \to \mathbb{R}^{d_z}$ and latent spates

$$z_0 = B(x_0), \qquad r_1 = B(x_1 - x_0).$$

Model conditional density:

$$p(r_1 \mid z_0, z_{-1}).$$

- Residuals improves accuracy: map is perturbation of identity.
- Historic state improves stability: B breaks Markovian structure.

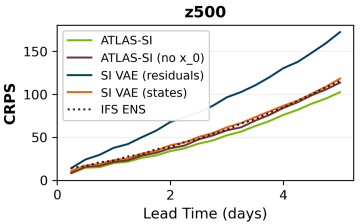
Decoder $D : \mathbb{R}^{d_z} \times \mathbb{R}^d \to \mathbb{R}^d$ approximately solves

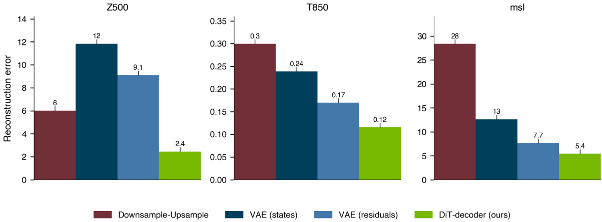
$$x_1 \approx x_0 + D(r_1, x_0).$$

Implementation

- B: bilinear interpolation to 181×360 equiangular grid (1.0 deg).
- D: Diffusion Transformer (DiT) with local attention (Natten).

Comparison to Autoencoders





Emperical Results

- Decoder only model gives more accurate reconstructions.
    - Learned latents contain high-frequency components.
- Rollout in learned latent space accumulates more error.
    - Latents have no temporal consistency.

Probabilistic Modeling Framework

Common Objective

Model latent conditional distribution $p(r_1 \mid z_0, z_{-1})$ via transport map

$$f_\theta : (\xi, z_0, z_{-1}) \to r_1.$$

Three Training Paradigms

Stochastic Interpolants

- Parameterize time-dependent drift term of a forward SDE.
- f_θ is solution operator of SDE.

Diffusion Models

- Parameterize time-dependent score of a data noising process.
- f_θ is solution operator of backward SDE/ODE.

CRPS-Based Generator

- f_θ is parametric transport map trained to minimize MMD variant.

Same transformer backbone supports all probabilistic formulations.

Diffusion Transformer Architecture

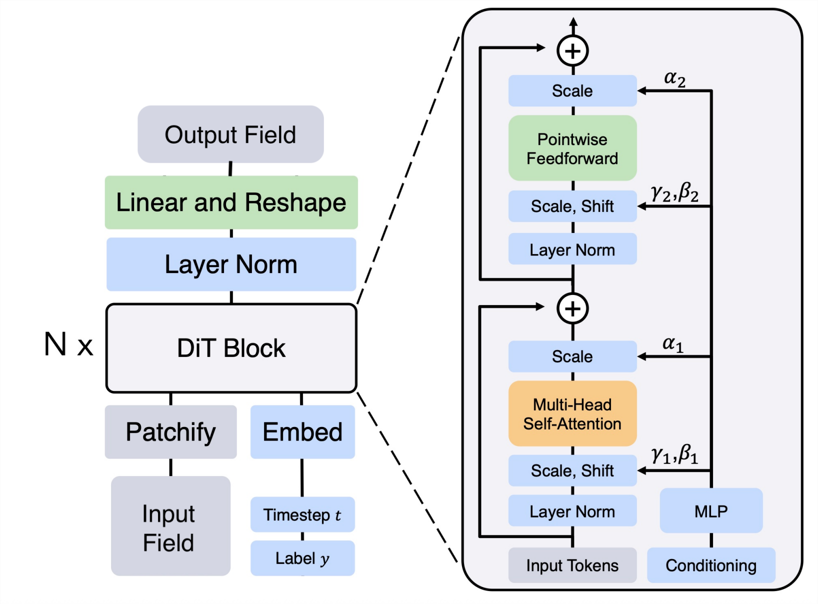


*Image adapted from Peebles, Xie, "Scalable Diffusion Models with Transformers." *International conference on computer vision.* 2023.

Stochastic Interpolants: Formulation

Interpolating Bridge Process

Define stochastic interpolant between z_0 and r_1

$$I_t = \alpha(t) z_0 + \beta(t) r_1 + \sigma(t) W_t, \quad t \in [0,1],$$

where W_t is a Wiener process and

$$\alpha(0) = 1,\ \alpha(1) = 0, \qquad \beta(0) = 0,\ \beta(1) = 1, \qquad \sigma(0) = \sigma(1) = 0.$$

Associated Forward SDE

The conditional law $\rho(r_1 \mid z_0, z_{-1})$ is recovered as terminal law of

$$dX_t = b(X_t, z_0, z_{-1} t)\, dt + \sigma(t)\, dW_t, \qquad X_0 = z_0.$$

Optimal drift minimizes

$$\int_0^1 \mathbb{E} \left| b(I_t, z_0, z_{-1}, t) - \dot{\alpha}(t) z_0 - \dot{\beta}(t) r_1 - \dot{\sigma}(t) W_t \right|^2 dt.$$

Chen et.al. "Probabilistic Forecasting with Stochastic Interpolants and Föllmer Processes." *PMLR.* 2024.

Stochastic Interpolants: Training and Sampling

Training Objective

Given samples $(z^\dagger_{j-1}, z^\dagger_j, r^\dagger_{j+1})$, minimize

$$\mathbb{E}_{t\sim U(0,1),\, \xi\sim\mathcal{N}(0,I)} \left| \hat{b}(I^\dagger_t, z^\dagger_j, z^\dagger_{j-1}, t) - \dot{\alpha}(t) z^\dagger_j - \dot{\beta}(t) r^\dagger_{j+1} - \dot{\sigma}(t)\sqrt{t}\xi \right|^2.$$

- Linear schedules for α, β, σ.
- Reparameterization ensures near-unit variance across t.

Sampling Procedure

Approximate SDE

$$d\hat{X}_t = \hat{b}(\hat{X}_t, z_0, z_{-1}, t)\, dt + \sigma(t)\, dW_t, \quad \hat{X}_0 = z_0.$$

- Discretize with first-order stochastic Runge–Kutta scheme.
- Terminal state $\mathrm{Law}(\hat{X}_1) \approx \mathrm{Law}(r_1 \mid z_0, z_{-1})$.

Diffusion Models: Formulation

Forward Noising Process

Define process

$$dX_t^F = \sqrt{2\sigma(t)\dot{\sigma}(t)}\, dW_t, \qquad X_0^F = r_1.$$

for σ non-negative and increasing. States z_0, z_{-1} remain fixed.

Reverse-Time SDE

Conditional law recovered from

$$dX_t = -2\sigma(t)\dot{\sigma}(t)\nabla_x \log p(X_t, z_0, z_{-1} t)\, dt + \sqrt{2\sigma(t)\dot{\sigma}(t)}\, d\bar{W}_t.$$

$\nabla_x \log p$ is score function of joint density.

- Reverse diffusion approximately transports Gaussian to $p(r_1 \mid z_0, z_{-1})$.
- Objective function for score given by Tweedie's formula

$$\int_0^T \mathbb{E}\big[|\nabla \log p(X_t^{\mathrm{F}}, z_0, z_{-1}, t) - \sigma(t)^{-2}(X_t^{\mathrm{F}} - r_1)|^2\big]\, dt.$$

Diffusion Models: Training and Sampling

Score Matching Objective

Given samples $(z_{j-1}^\dagger, z_j^\dagger, r_{j+1}^\dagger)$, minimize

$$\mathbb{E}_{t,\xi} \left| \hat{s}(r_{j+1}^\dagger + \sigma(t)\xi, z_j^\dagger, z_{j-1}^\dagger, t) - \sigma(t)^{-1}\xi \right|^2 .$$

- Log-normal sampling of noise level σ.
- Reparameterization ensures near-unit variance across t.

Sampling Procedure

Approximate backward SDE

$$d\hat{X}_t = -2\sigma(t)\dot{\sigma}(t)\hat{s}(\hat{X}_t, z_0, z_{-1}t)\,dt + \sqrt{2\sigma(t)\dot{\sigma}(t)}\,d\bar{W}_t.$$

- Second order predictor-corrector method based on Heun.
- Non-uniform time grid with step sizes proportional to σ.

Karras et.al. "Elucidating the Design Space of Diffusion-Based Generative Models." NeuIPS. 2022.

CRPS-Based Generator: Formulation

Direct Conditional Transport Map

Learn deterministic transport map

$$f_\theta : (\xi, z_0, z_{-1}) \mapsto r_1, \qquad \xi \sim \mathcal{N}(0, I_p).$$

such that

$$f_\theta(\cdot, z_0, z_{-1})_\sharp N(0, I_p) \approx p(r_1 \mid z_0, z_{-1}).$$

CRPS Objective

Minimize energy-score

$$\mathbb{E}\left[|f_\theta(\xi, z_0, z_{-1}) - r_1| - \frac{1}{2} |f_\theta(\xi, z_0, z_{-1}) - f_\theta(\xi', z_0, z_{-1})| \right].$$

- First term: forecast accuracy.
- Second term: ensemble diversity.
- Equivalent to MMD with p.s.d. kernel $k(x, y) = -|x - y|$.

Lang et.al. "AIFS – ECMWF's data-driven forecasting system." arXiv:2406.01465. 2024.

CRPS Generator: Training & Spectral Regularization

Training Objective

Given samples $(z^\dagger_{j-1}, z^\dagger_j, r^\dagger_{j+1})$, minimize

$$|f_j(\xi) - r^\dagger_{j+1}| + |f_j(\xi') - r^\dagger_{j+1}| - |f_j(\xi) - f_j(\xi')|$$

where $f_j(\xi) = f_\theta(\xi, z^\dagger_j, z^\dagger_{j-1})$ with 2 ensemble members $\xi, \xi' \sim N(0, I_p)$.

CRPS alone may:

- Under-represent high-frequency modes.
- Be unstable during training due to low ensemble size.

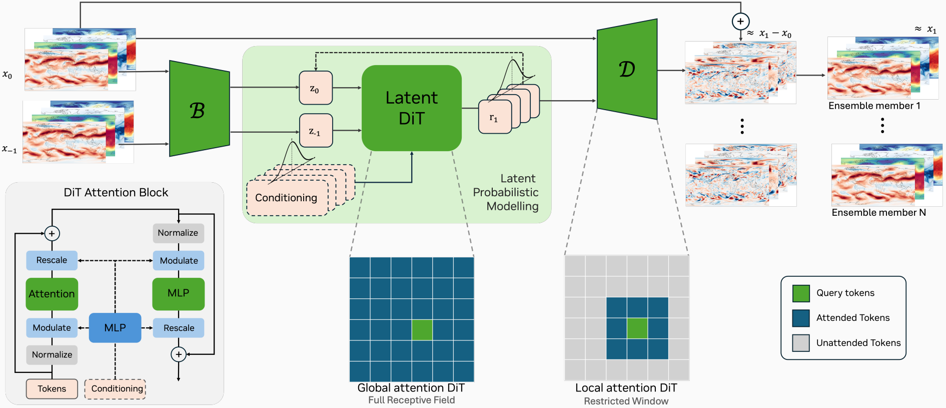
Add spectral term, for $\hat{S}$ spherical harmonic transform,

$$|\hat{S}(f_j(\xi)) - \hat{S}(r^\dagger_{j+1})| + |\hat{S}(f_j(\xi')) - \hat{S}(r^\dagger_{j+1})| - |\hat{S}(f_j(\xi)) - \hat{S}(f_j(\xi'))|$$

Sampling Procedure

Single network evaluation orders of magnitude faster than discrete SDE.

Overview of Methodology



Training, Sampling & Metrics

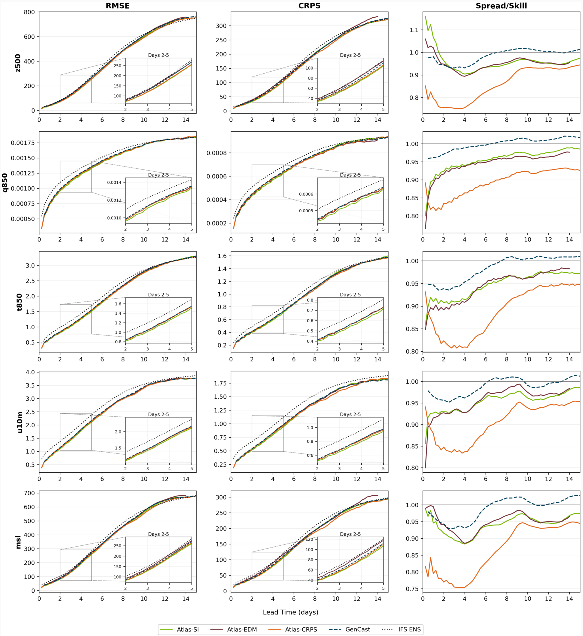
Training

- ERA5 fields Gaussian normalized per-variable (separate states and residuals).
- Additional conditioning fields: cosine-zenith angle, land-sea mask, surface geopotential.
- White noise sampled on spherical harmonic basis (KL expansion).
- Trained with 32 H100 GPUs with hard-restart damped cosine decay.
- 2×3 patch size and embedding dim $e = 3328$ (2.5B parameters).

Sampling and Metrics

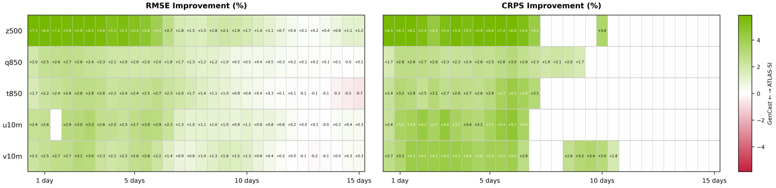
- SDEs discretized with 100 time steps (44s inference time).
- Evaluation based on 56 ensemble members with metrics: RMSE of mean, CRPS, skill-spread ratio.
- Using per date statistics, paired t-test used to indicate statistical significance.

Fifteen Day Rollout Results

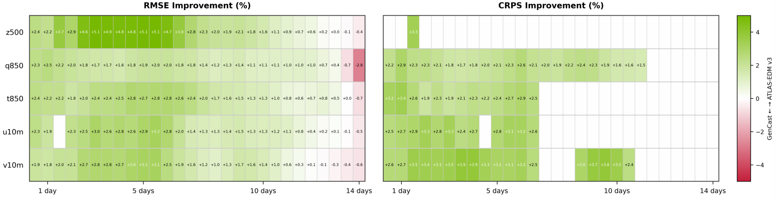


Score card vs IFS

Score card vs GenCast



White cells: not significant (p ≥ 0.05)



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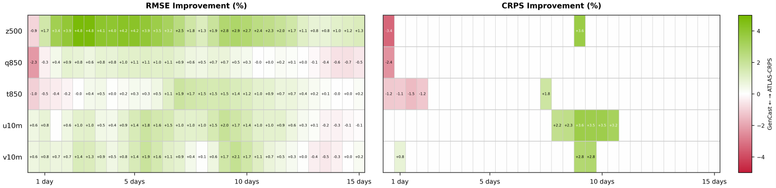
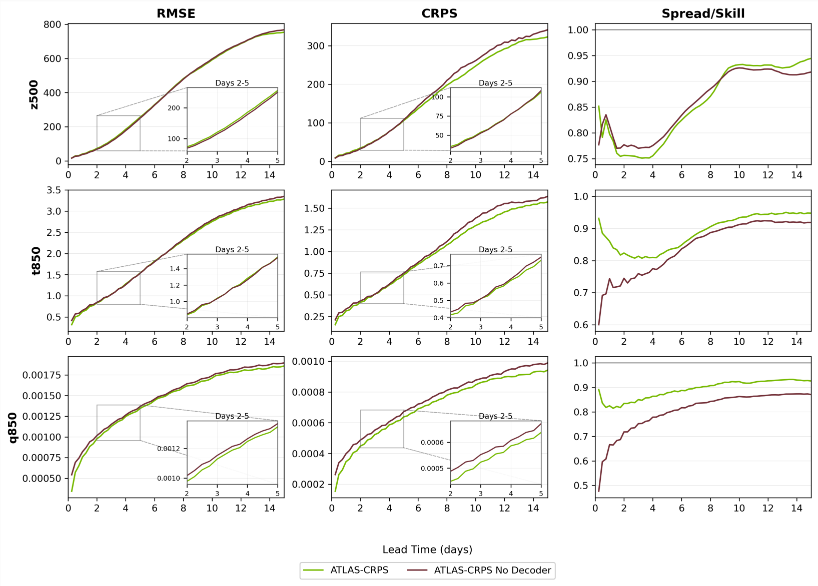
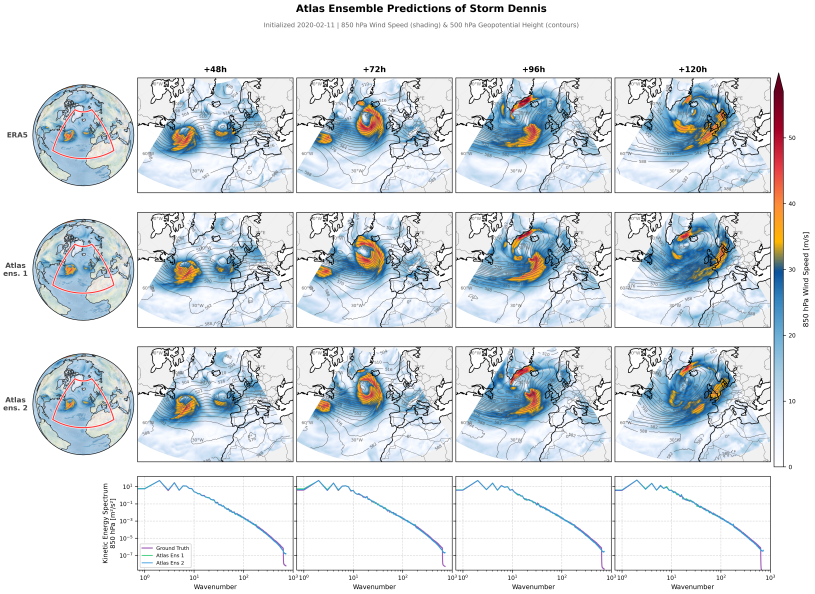


White cells: not significant (p ≥ 0.05)

Role of the Decoder



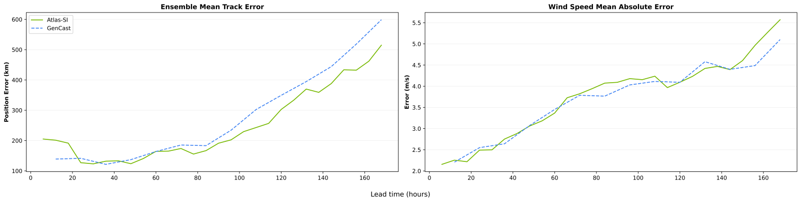
Spectral Analysis: Storm Dennis

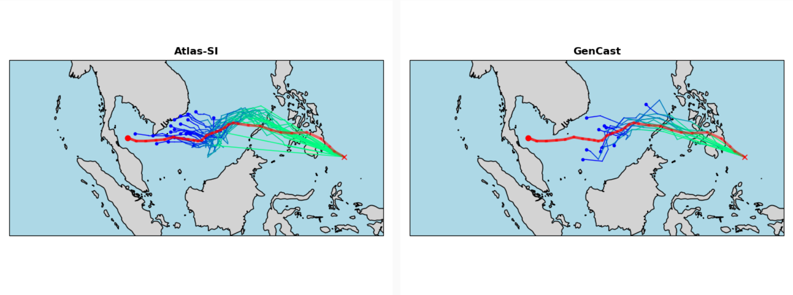


Atlas Ensemble Predictions of Storm Dennis

Initialized 2020-02-11 | 850 hPa Wind Speed (shading) & 500 hPa Geopotential Height (contours)

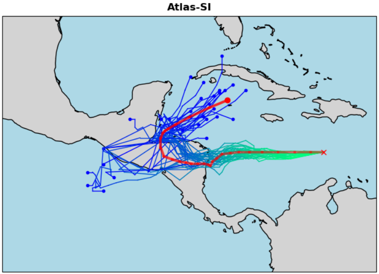
Cyclone Tracking



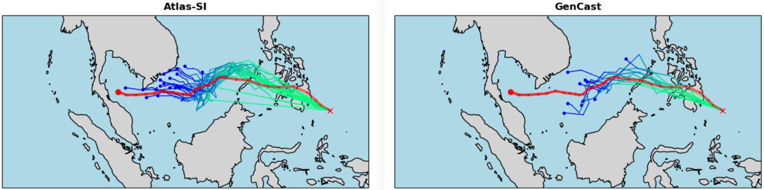


Tropical Storm Krovanh 7 day track, initialized December 17, 2020 UTC 12:00.

Cyclone Tracking Examples



Hurricane Eta 7 day track, initialized October 31, 2020 UTC 18:00.



Tropical Storm Krovanh 7 day track, initialized December 17, 2020 UTC 12:00.

Conclusion

Key Result

Latent transformer framework achieves state-of-the-art probabilistic forecasts.

Technical Insight

Architecture robustness across stochastic interpolants, diffusion, and CRPS training.

Open Questions

Physics constraints, conservation laws, training on ensemble data, long-term stability.