

# A Regime-Aware Trajectory Prediction Framework for 1000+ Systems Biology Models

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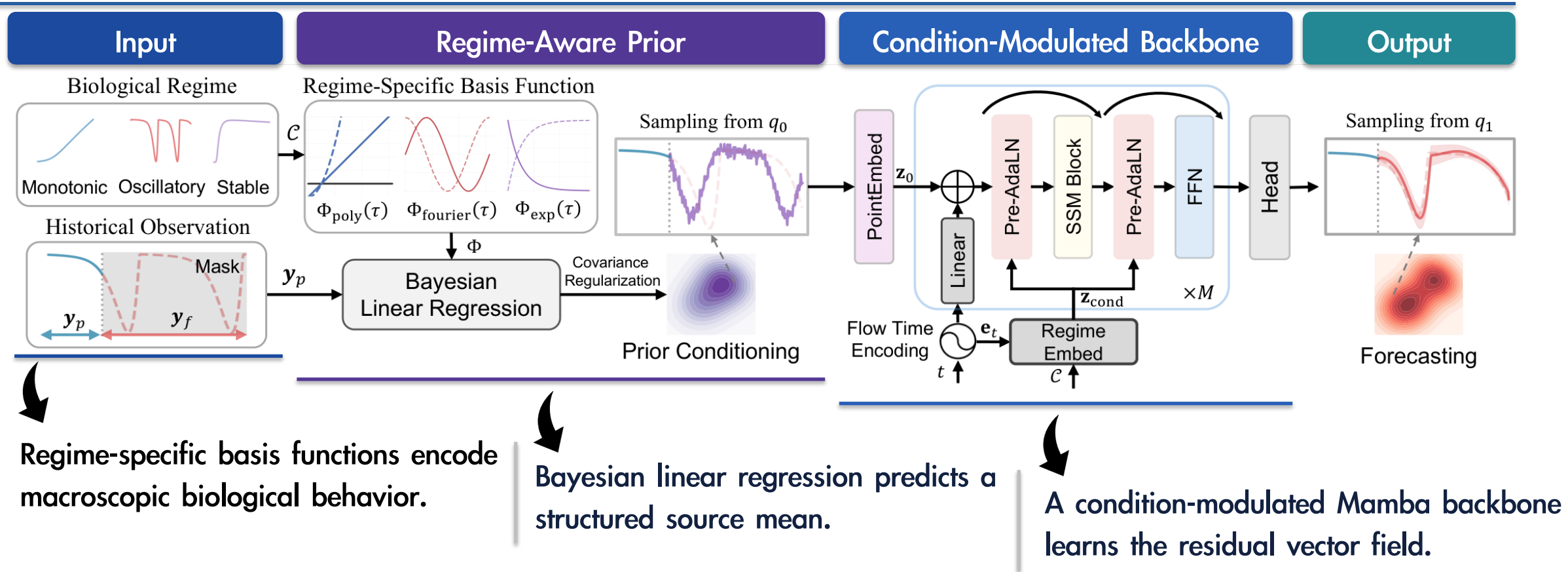


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# Core Idea: Replace Gaussian Noise with a Biological Prior



Standard Flow Matching

$$q_0 = \mathcal{N}(0, I)$$

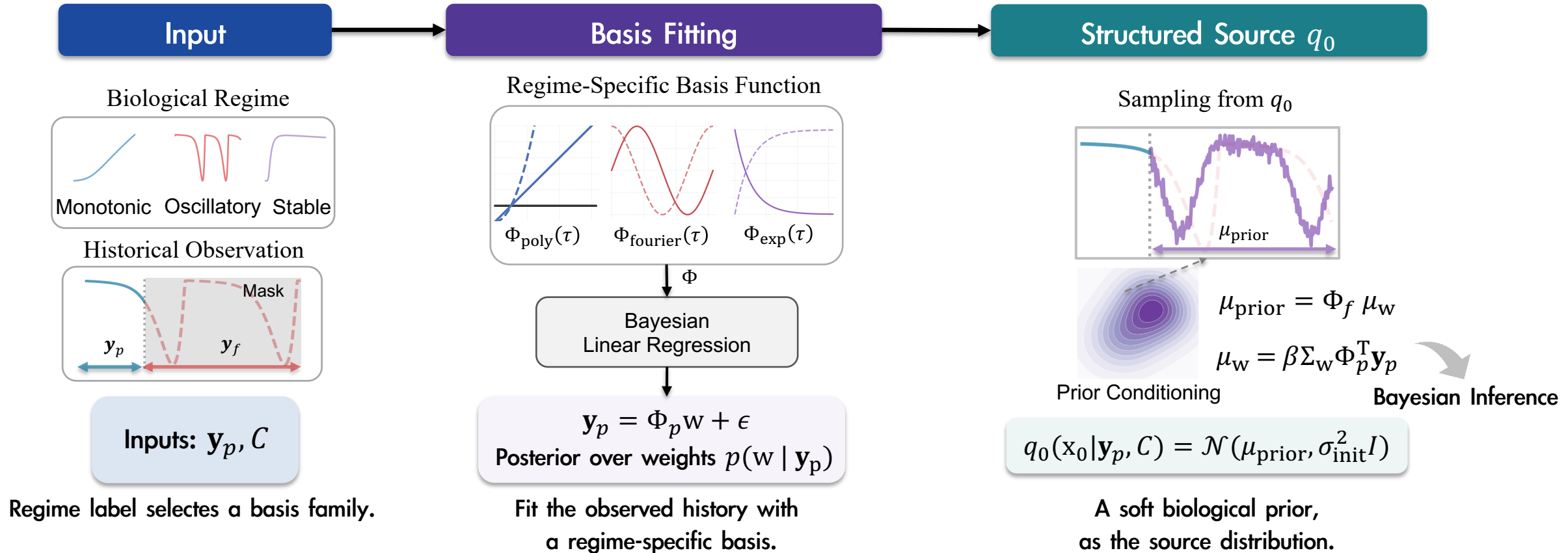
Random Noisy

RegimeFlow

$$q_0(\mathbf{x}_0 | \mathbf{y}_p, C) = \mathcal{N}(\mu_{\text{prior}}(\mathbf{y}_p, C), \sigma_{\text{init}}^2 I)$$

Biological Plausible future

# Zoom-in: From Regime and History to Structured Souce $q_0$



**Bayesian Inference:**

$$\mu_{prior} = \Phi_f \mu_w,$$

$$\mu_w = \beta \Sigma_w \Phi_p^T y_p$$

Instead of starting from Gaussian noise,  
RegimeFlow initializes flow matching from a biologically source distribution

# SysBio-Traj Benchmark: Cross-System Biological Forecasting



## SysBio-Traj Benchmark



1,050 biological systems



Trajectory-level Regime Annotation



Reproducible Python benchmark package

### Diversity Overview



Human



Mouse



Plant



Yeast

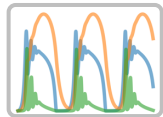


Virus

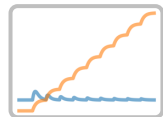
### Trajectory Regime Labels



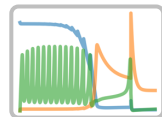
Stable



Oscillatory



Monotonic



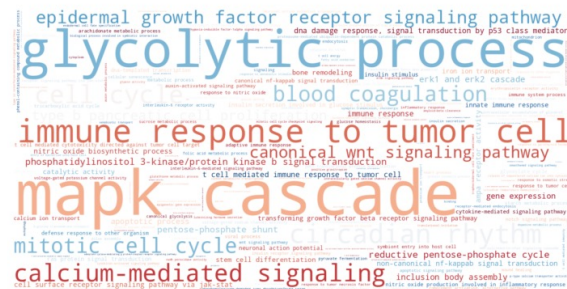
Complex

## Diverse Organisms and Pathway

### Diverse Organisms



### Diverse Pathway

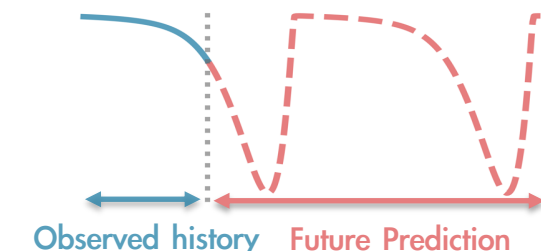


## Forecasting Task

### Cross System prediction



### Trajectory Prediction

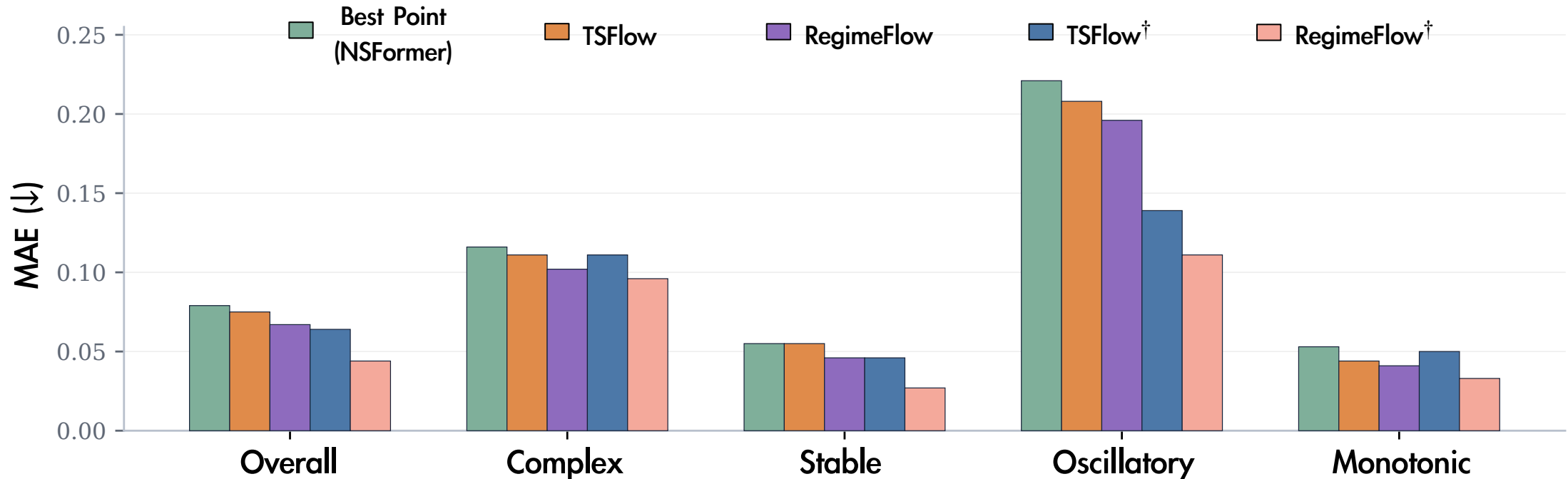


Long-horizon extrapolation from short observations



The goal is not to fit one system, but to generalize long-horizon forecasting to unseen biological systems.

# Main Results: Better Accuracy and Calibration



Point Accuracy

**25% ↓ MSE**

vs. strongest baseline

Point Accuracy

**31% ↓ MAE**

vs. strongest baseline

Probabilistic Quality

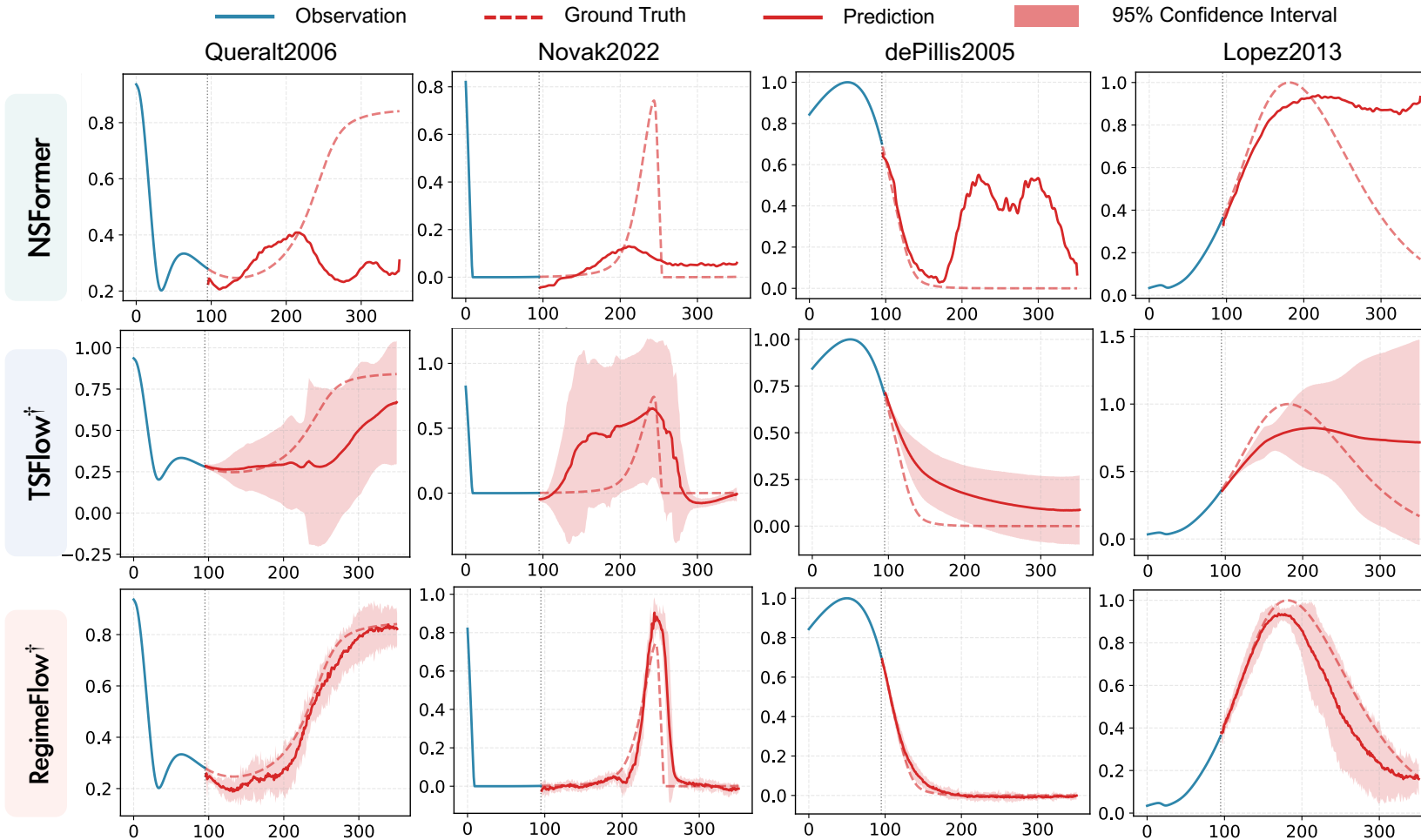
**17% ↓ CRPS**

Better calibration



RegimeFlow consistently improves both deterministic accuracy and uncertainty quality by starting from biologically priors.

# Qualitative Forecasts: Accurate and Calibrated Trajectories



✓ Tracks regime structure

Capture oscillation, convergence and complex trends.

✓ Calibrated uncertainty

Confidence bands remain informative, not overly diffuse.

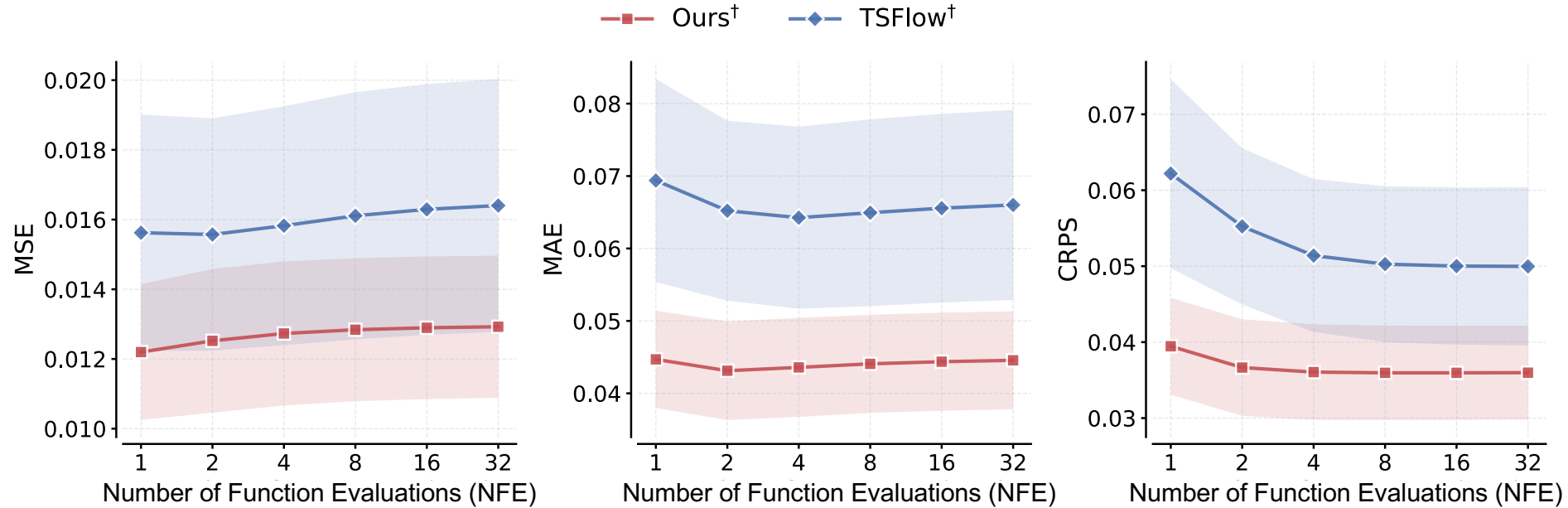
✓ Robust to unseen systems

Generalizes beyond biological systems observed during training.



Regime-aware priors help the model follow biological trajectory shapes while maintaining informative uncertainty bands.

# Efficient Probabilistic Forecasting with One-Step Inference



**NFE=1**

one-step generation



**7.7 ms/sample**

Fast probabilistic inference



**9.3× faster**

than TSFlow



A better source distribution enables accurate uncertainty estimation  
with **one function evaluation.**

# Conclusion: RegimeFlow Enables Cross-System Biological Forecasting



SysBio-Traj Benchmark



1,050 biological systems



Trajectory-level Regime Annotation



Reproducible Python benchmark package

Diversity Overview



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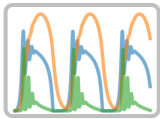


Virus

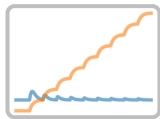
Trajectory Regime Labels



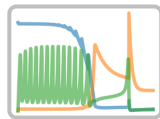
Stable



Oscillatory



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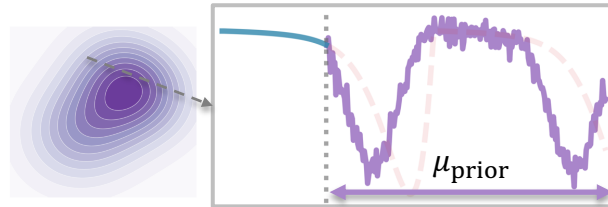
Complex



RegimeFlow Framework



Sampling from  $q_0$

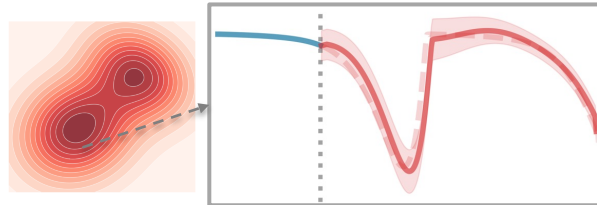


Prior Conditioning



Condition-Modulated Backbone

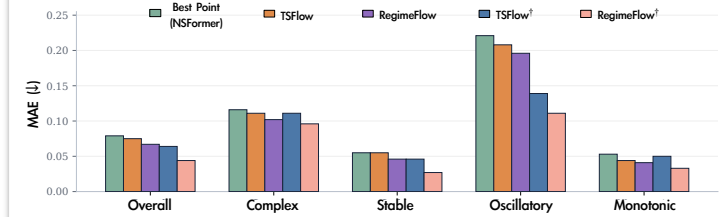
Sampling from  $q_1$



Forecasting

Empirical Gains

Main Results



MSE Across Major Biological System Taxonomies

