Uncertainty-aware Surrogate Models for Airfoil Flow Simulations with Denoising Diffusion Probabilistic Models

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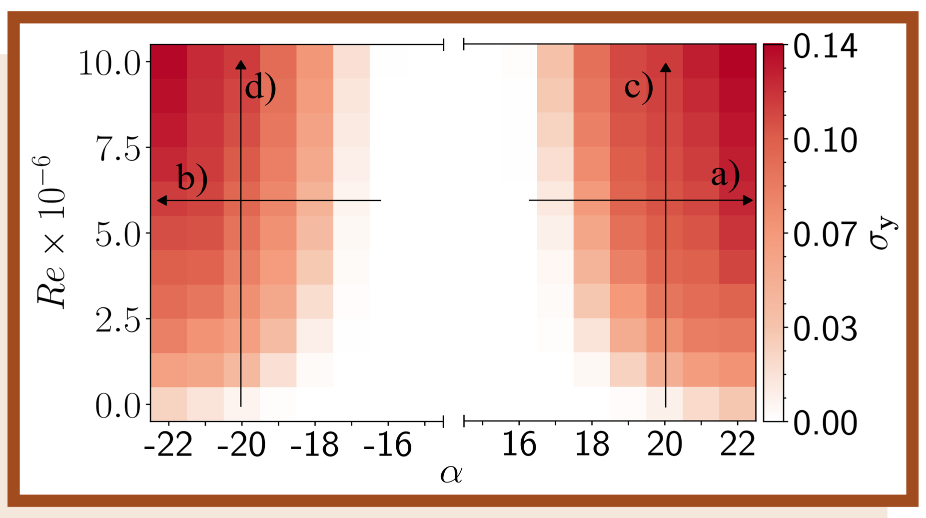
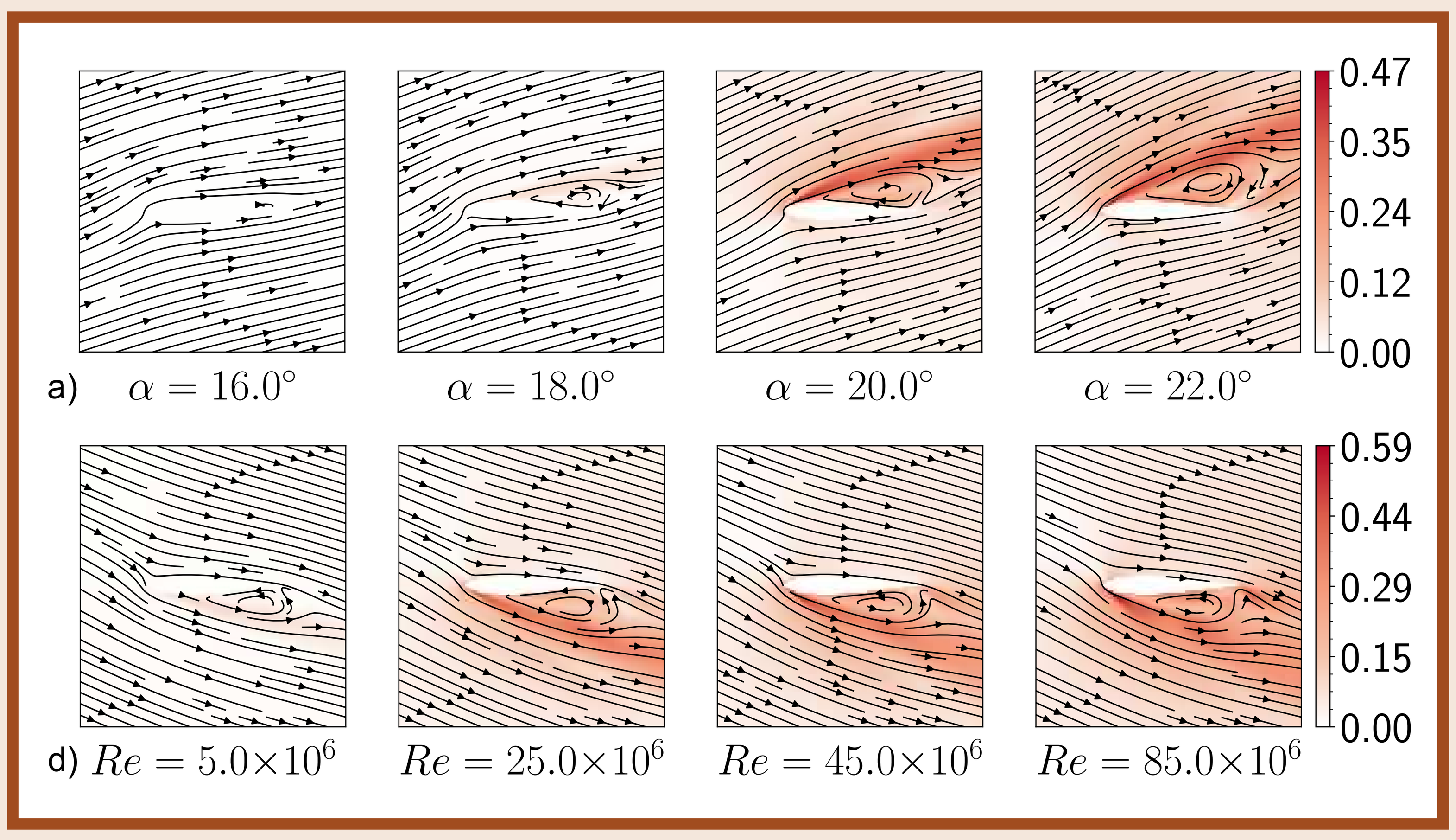
Motivations

Turbulence simulations contain many **uncertainties**, which usually change with different control parameters.



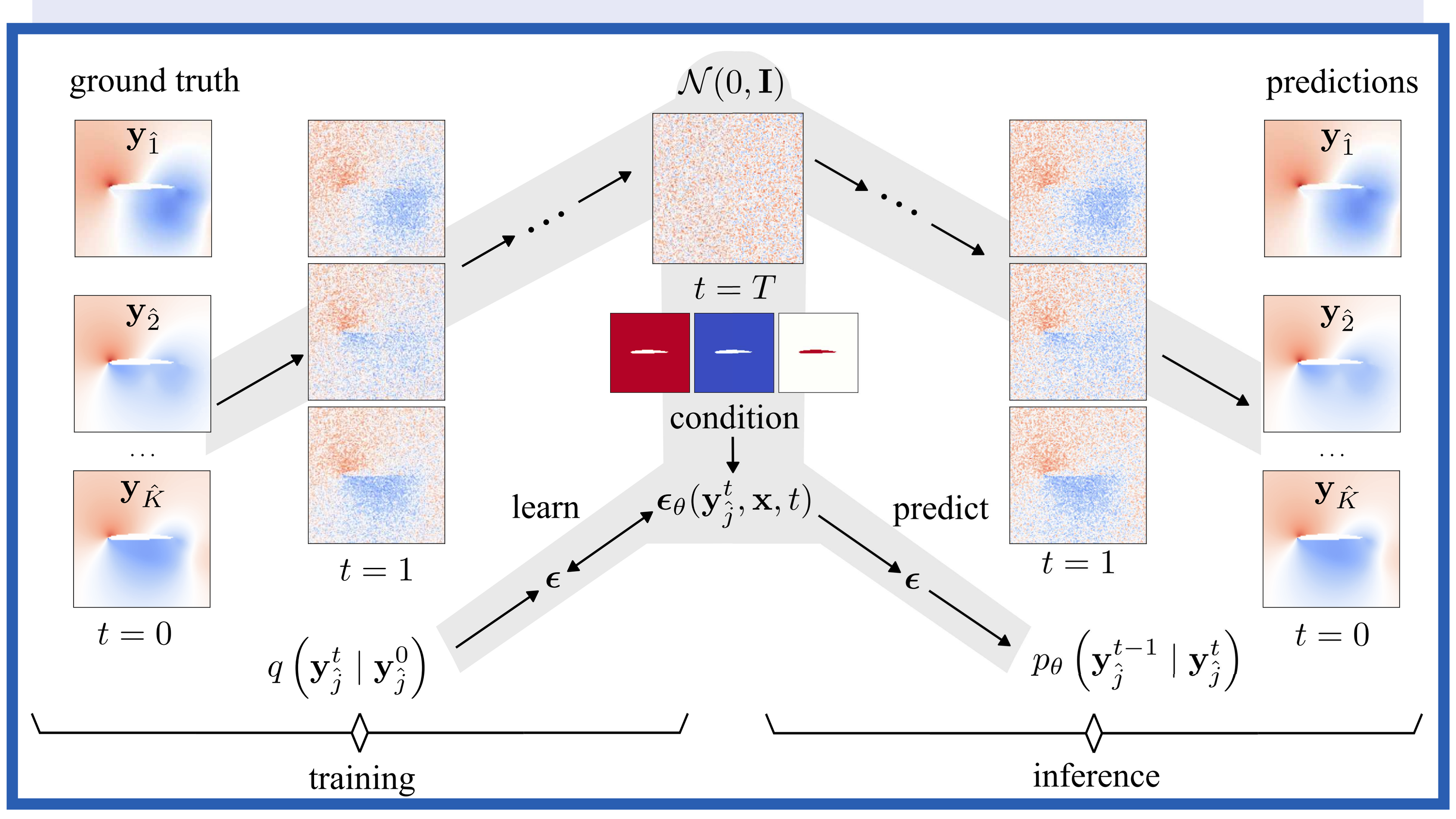
For example, the uncertainty in the simulation of airfoil flows is highly related to the **airfoil shape**, **Reynolds number (Re)**, and **angle of attack (α)**. When dealing with a specific airfoil shape, the uncertainty tends to escalate as the Reynolds number and angle of attack increase.

Capturing these uncertainties is essential for developing a **reliable** deep surrogate model for turbulence simulation. This study uses **Denoise Diffusion Probabilistic Models (DDPMS)** to build an **uncertainty-aware** surrogate model for airfoil flow simulations.



DDPMs

The core of building an uncertainty-aware surrogate model is to enable a **probabilistic** output of the surrogate model and learn the **data distribution**. DDPMs first learn a forward Markov chain of transforming the data distribution into a simple Gaussian distribution by adding **Gaussian noise** to the samples from data distribution step by step. With the learned forward chain, DDPMs can generate samples belonging to the original data distribution by step-by-step **denoising** a sample from the standard Gaussian distribution.



Baselines

We introduce **Bayesian Neural Networks (BNNs)** and the **heteroscedastic model** (Gaussian mixture models) as baselines to compare with DDPM. BNN assumes a **Gaussian prior** for the neural network's parameter. During the training procedure, BNNs try to force the distribution of the neural network close to the priori and learn from the dataset simultaneously:

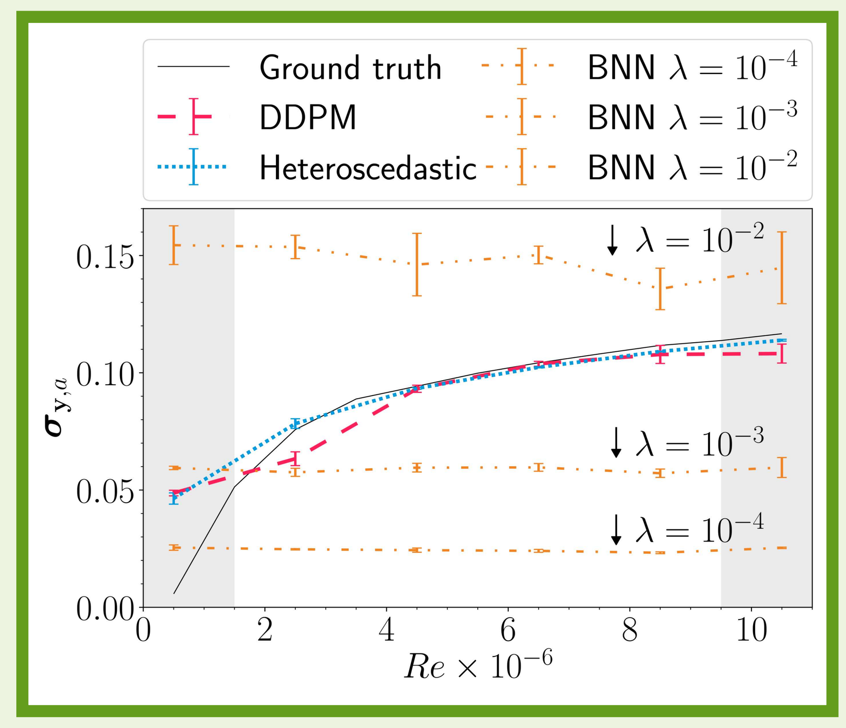
$$\mathcal{L}_{\rm NN}(\phi) = \underbrace{\lambda \mathrm{KL}(q_\phi(\theta)||\underbrace{p(\theta)}_{\text{prior}})}_{\text{uncertainty related}} - \underbrace{\mathbb{E}_{q_\phi}[\log(p(\mathbf{d}|\theta))]}_{\text{learn from data}}$$

Meanwhile, the **heteroscedastic model** assumes a **Gaussian distribution** of the **data** and predicts the mean(μ_θ) and standard deviation(σ_θ) through maximum posterior probability inference:

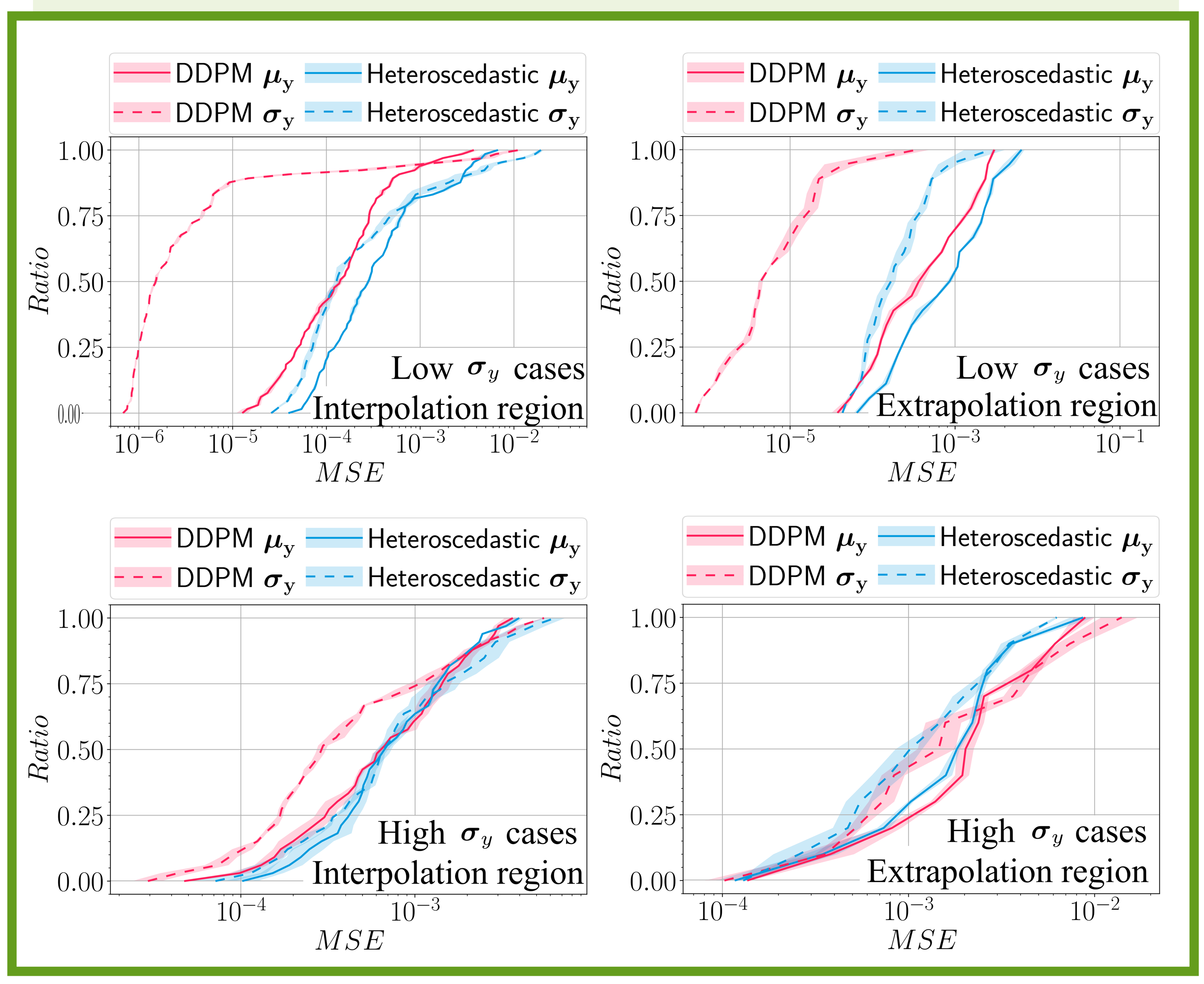
$$\mathcal{L}_{\rm NN}(\theta) = \frac{1}{N}\sum_{i=1}^{N}\left[\frac{1}{2[\sigma_{\theta,\mathbf{y}}(\mathbf{x})]^2}\|\mathbf{y}_i - \mu_{\theta,\mathbf{y}}(\mathbf{x})\|^2 + \frac{1}{2}\log[\sigma_{\theta,\mathbf{y}}(\mathbf{x})]^2\right]$$

Accuracy

We compare the performance of DDPM with BNN and the heteroscedastic model. For prediction accuracy, the **BNN** can **not** accurately predict the uncertainty of the flow field as it is highly limited by the **Gaussian assumption** of the prior distribution and the **λ coefficient** controlling the uncertainty of the network.

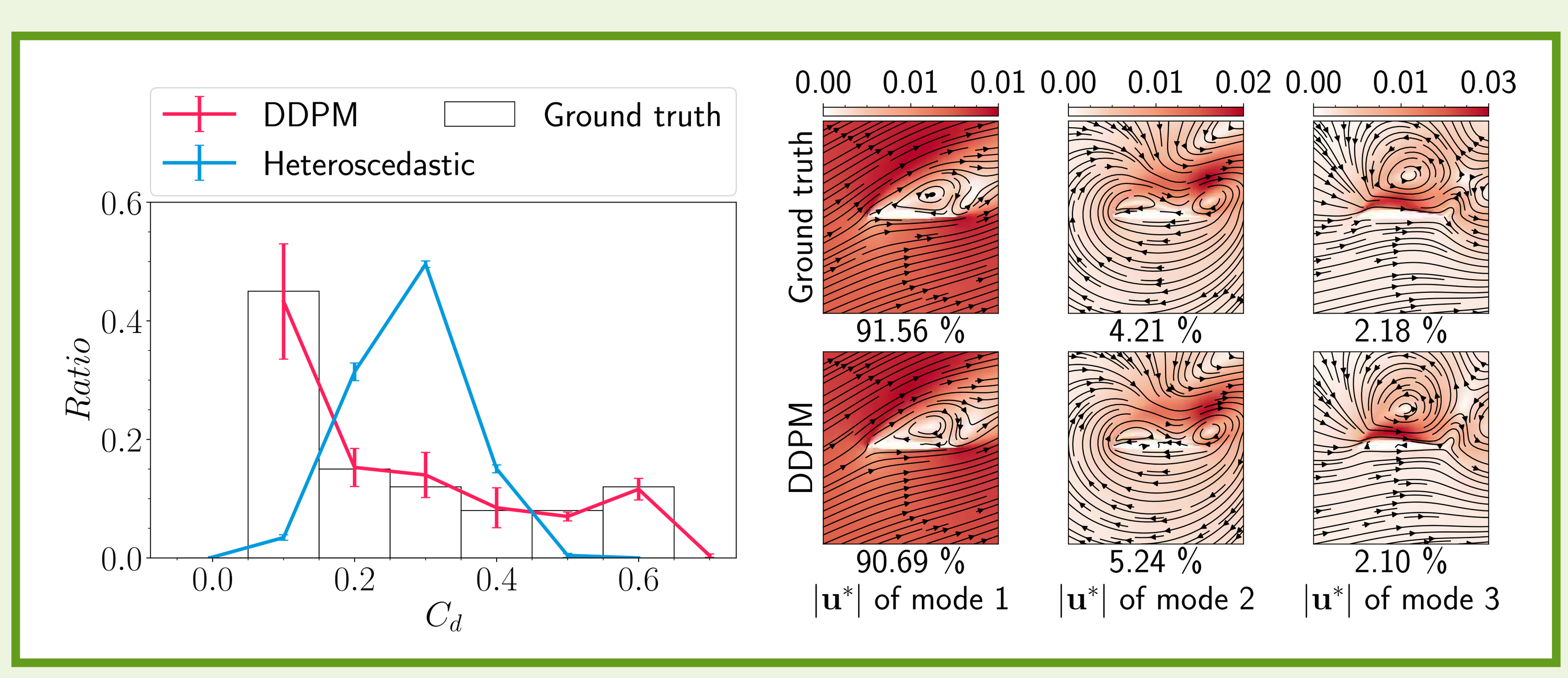


Although both the heteroscedastic and DDPM can give accurate predictions on uncertainty, **DDPM** generally has a **higher accuracy**.



Learned distribution

Although the **heteroscedastic model** can also provide accurate uncertainty predictions regarding the standard deviation, it is still limited by its **Gaussian distribution assumption** of the data. While the **DDPM** model does **not** rely on any assumptions, it can reconstruct the **whole distribution** accurately rather than just predict the moments of the distribution.



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Related works
Uncertainty-Aware Surrogate Models for Airfoil Flow Simulations with Denoising Diffusion Probabilistic Models, Qiang Liu and Nils Thuerey, AIAA Journal, 2024
https://github.com/tum-pbs/Diffusion-based-Flow-Prediction