Enhancing Surrogate Modeling for Turbidity Currents via Super-Resolution with Diffusion Models

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Introduction: Data-driven Parametric Surrogate Model

Data-driven Parametric Surrogate models[1,2] help us on:

- 🙂 Reduce the computational cost of forward evaluations in high-fidelity models.
- 🙂 (+) Data-driven: allows a non-intrusive implementation.
- 🙂 (+) Parametric: Enable efficient *many-query* analyses, such as uncertainty quantification (UQ).
- ☹️ **Trade-off**: reduced solution accuracy.

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[1] Guo, Hesthaven - Data-driven reduced order modeling for time-dependent problems. Computer Methods in Applied Mechanics and Engineering, vol. 345, 2018.

[2] Fresca, Manzoni - Pod-dl-rom: Enhancing deep learning-based reduced order models for nonlinear parametrized pdes by proper orthogonal decomposition. Computer Methods in Applied Mechanics and Engineering, vol. 388, 2022.

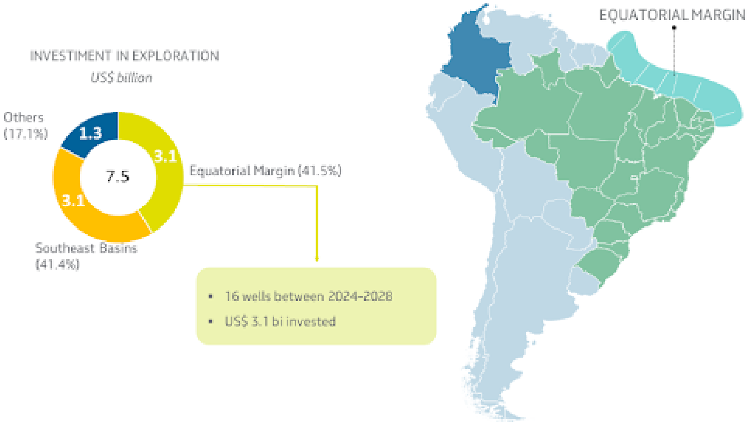
Introduction: Super-Resolution in Surrogate Models

🎯 **Goal of Super-Resolution**: Enhance image quality by reconstructing finer details.

- **Proposed Approach**: Apply super-resolution techniques to improve the quality of predictions generated by a surrogate model.
- **Training Strategy**:
  - Train super-resolution model on the same dataset as the surrogate model.
  - Leverage high-quality data to boost surrogate model output fidelity.

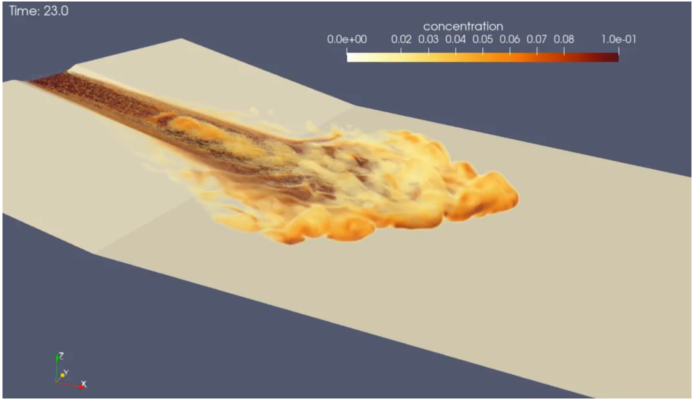
🏆 **Expected Outcome**: Improved accuracy and visual quality in surrogate model predictions.

Motivation: Prediction of Sediment Deposition



Sediment deposition is a key aspect for geologists - Oil Extraction!

Motivation: Prediction of Sediment Deposition



We measure the concentration at the bottom of the basin.

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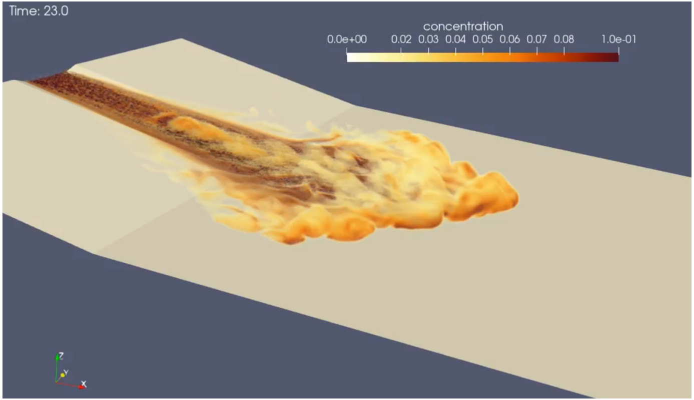
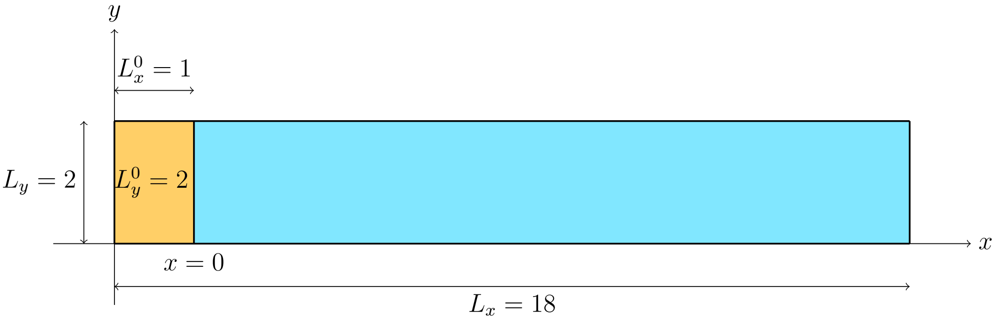


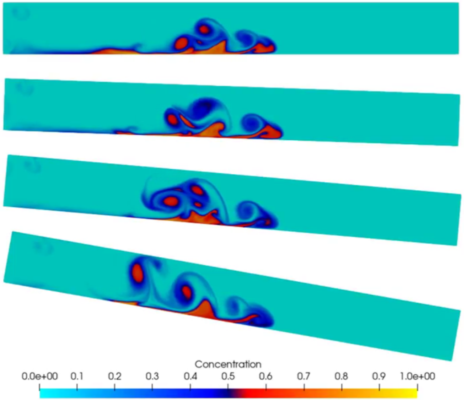
We measure the concentration at the bottom of the basin.

Target: Layers of deposition material.

ROM for Turbidity Currents under Lock-Exchange Setup



Lock-Exchange Setup in 2D



Evolution of Concentration.

Governing Equations

Navier–Stokes equations in non-dimensional form in their non-conservative formulation:

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\nabla p + \frac{1}{\sqrt{Gr}} \Delta \boldsymbol{u} + c\, \boldsymbol{e}_\theta^g, \tag{1a}$$

$$\nabla \cdot \boldsymbol{u} = 0, \tag{1b}$$

$$\frac{\partial c}{\partial t} + \left(\boldsymbol{u} + u_S\, \boldsymbol{e}_\theta^g \right) \cdot \nabla c = \nabla \cdot \left(\frac{1}{Sc\sqrt{Gr}} \nabla c \right). \tag{1c}$$

- Domain: $\Omega = [0, 18] \times [0, 2]$
- BC: no-slip condition ($\boldsymbol{u} = \mathbf{0}$) on all solid boundaries
- BC: zero-flux Neumann condition for sediment concentration
- ICs: $c = 1$ for $x < 0$ and $c = 0$ Ow.,

- c: normalized sediment concentration
- $\boldsymbol{u}$: velocity field, u_s: cte. sedimentation vel.
- $Gr = \sqrt{5} \times 10^3$ Grashof, $Sc = 1.00$ Schmidt
- p: pressure, θ: channel's inclination angle
- Gravit. force: $c\, \boldsymbol{e}_\theta^g$, $\boldsymbol{e}_\theta^g = (\sin\theta, -\cos\theta)$

Dataset Generation

Simulation Setup - Full Order Model (FOM):

- Stabilized FEM - residual-based var. multiscale method[1] - FEniCS framework
- $\Omega = [0, 18] \times [0, 2]$, 701×101 nodes, yielding 70801 concentration values.
- Time interval $[0, 22]$ with timestep $\Delta t = 0.01$.;
- Concentration snapshots every 0.05 time units, giving 440 snapshots.

Data Generation:

- Angles of $0, 2, 4, 6, 8, 10$ for training the ROM Model;
- Angles of 5 and 12 for testing - interpolation and extrapolation.

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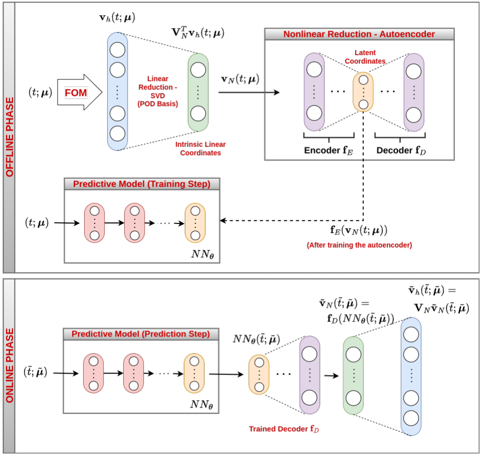
[1] G. Guerra, S. Zio, J. Camata, F. Rochinha, R. Elias, P. Paraizo, and A. Coutinho - **Numerical simulation of particle-laden flows by the residual-based variational multiscale method** - International Journal for Numerical Methods in Fluids, 2013.



Reduced-order Model (ROM) Setup

[1] R. Velho, A. Côrtes, G. Barros, F. Rochinha. A. Coutinho - **Advances in Data-Driven Reduced Order Models using Two-Stage Dimension Reduction for Coupled Viscous Flow and Transport** - Preprint: https://papers.ssrn.com/sol3/papers.cfm?abstract_id=5064259 , 2024.

Denoising Diffusion Probabilistic Model (DDPM)

Overview:

- DDPMs are generative models that generate data by reversing a gradual noise-adding process.
- Data is iteratively corrupted with Gaussian noise, then reconstructed by learning a denoising sequence.

Key Concepts:

- **Forward Process**: Gradually adds noise to data to create a noisy sequence.
- **Reverse Process**: Learns to remove noise, restoring the original data from a noisy state.
- **Applications**: High-quality image generation, **super-resolution**, inpainting, and more.

Denoising Diffusion Probabilistic Model (DDPM)

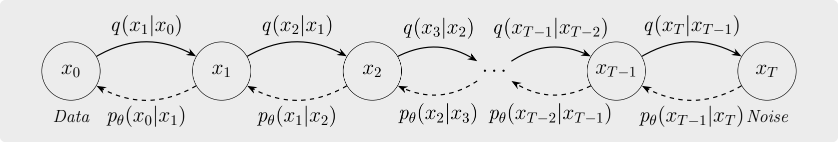


Figure: Markovian process in DDPM showing forward diffusion q and reverse denoising p_θ transitions.

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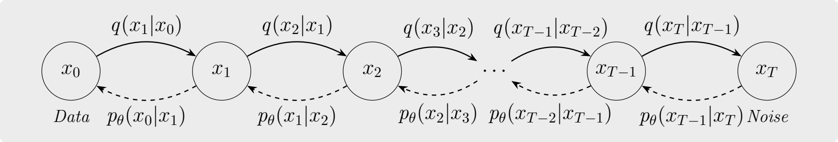


Figure: Markovian process in DDPM showing forward diffusion q and reverse denoising p_θ transitions.

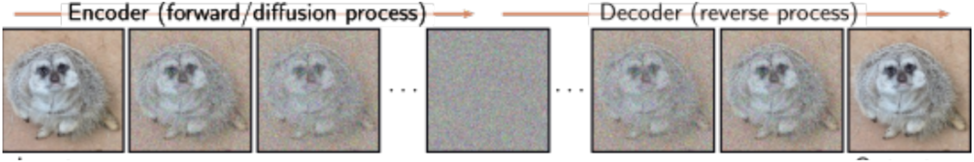


Figure: S.J.D. Prince, *Understanding Deep Learning*, The MIT Press, 2023.

Forward Diffusion (Encoder) Process in DDPM

Overview:

- Gradually adds Gaussian noise to data over T steps, transforming data into near-random noise.
- Enables learning of the data distribution through progressive noise addition.

Mathematics:

- Transition: $q(x_t|x_{t-1}) = \mathcal{N}(x_t; \sqrt{1-\beta_t} \cdot x_{t-1}, \beta_t I)$
- After t steps: $q(x_t|x_0) = \mathcal{N}(x_t; \sqrt{\bar{\alpha}_t} \cdot x_0, (1-\bar{\alpha}_t) I)$
- $\beta_t \in [0, 1]$: noise schedule, $\alpha_t = 1 - \beta_t$, $\bar{\alpha}_t = \prod_{s=1}^{t} \alpha_s$

Result:

- Produces noisy images $\{x_1, x_2, ..., x_T\}$, which the reverse model learns to denoise.

Reverse Process (Decoder) and Loss in DDPM

Reverse Process:

- Removes noise added in the forward process, reconstructing data from noise.
- Modeled as: $p_\theta(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \sigma_t^2 I)$, $\{\sigma_t^2\}$ predetermined.

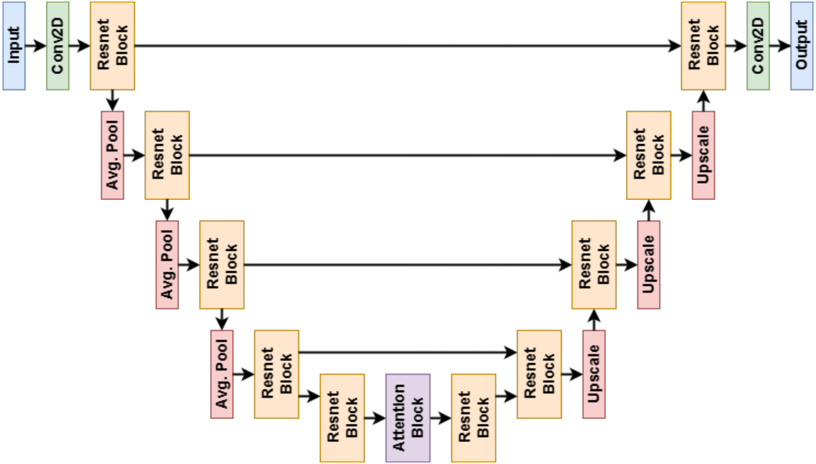
Neural Network Architecture:

- U-Net with skip connections is used to predict $\mu_\theta(x_t, t)$, as it efficiently captures multi-scale information, refining noise to match the original data structure.

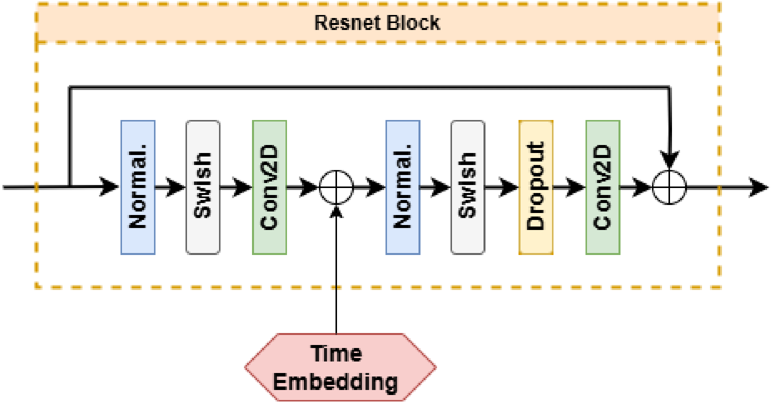
Loss Function:

- Minimize the noise prediction error: $\mathcal{L}_{\text{DDPM}} = \mathbb{E}_{t,\epsilon}\left[\|\epsilon - \epsilon_\theta(x_t, t)\|^2\right]$.
- Trains model ϵ_θ to accurately predict and remove noise step-by-step.

Super-Resolution U-net Architecture



The Resnet Block



Super-Resolution: Training Setup

- **GPU**: NVIDIA RTX A4000 (16MB RAM)
- **Framework**: PyTorch with Adam optimizer
- **Epochs**: 300 (approx. 16 hours)
- **Learning Rate**: Fixed at 2×10^{-4}
- **Batch Size**: 12
- **Number of diffusion time steps**: 1000
- **Linear schedule for β_t: from $\beta_1 = 10^{-4}$ to $\beta_{1000} = 0.02$**

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[1] D. Shu, Z. Li, A. Farimani - **A physics-informed diffusion model for high-fidelity flow field reconstruction** - Journal of Computational Physics, 2023.

[2] D. Shu, Z. Li, A. Farimani - **Diffusion-based-Fluid-Super-resolution** - https://github.com/BaratiLab/Diffusion-based-Fluid-Super-resolution/tree/main_v1.

Applying the trained SR model:

- For evaluation, we applied the trained diffusion super-resolution model to the ROM outputs for angles not included in the training set;

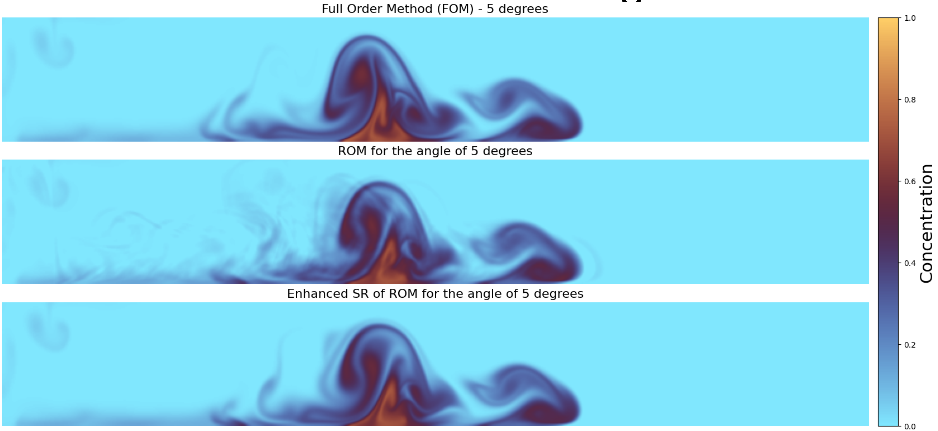
- ROM output is not Gaussian noise; it still contains the principal characteristics expected in the final solution;

- Thus we cannot input the ROM at the final step of the diffusion chain (1000) for denoising. We must introduce it at an intermediate step $n_s < 1000$;

Applying the trained SR model:

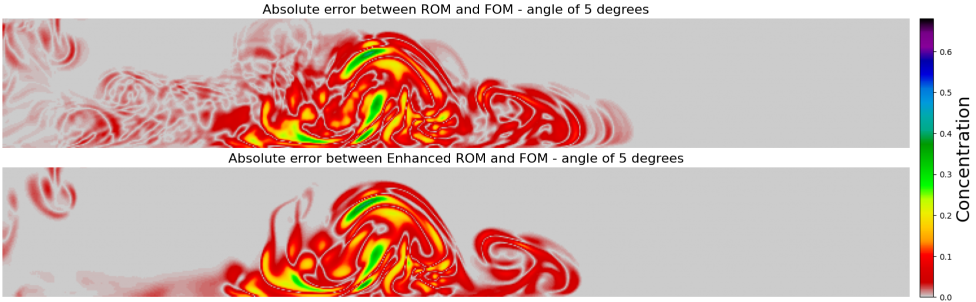
- When the selected starting time is insufficient, the Enhanced ROM results exhibit numerous numerical artifacts, indicating inadequate denoising;
- Conversely, an excessively large starting time can lead to overcorrection, potentially eliminating smaller secondary dynamics and resulting in information loss;
- Through empirical testing, we determined that a starting time of $n_s = 200$ **produces optimal reconstruction quality**;
- Computational Time: 1 time/image - 10s. Entire dynamics (440 times) - 27 minutes.

Visual of the reconstruction - θ=5 degrees at 20s



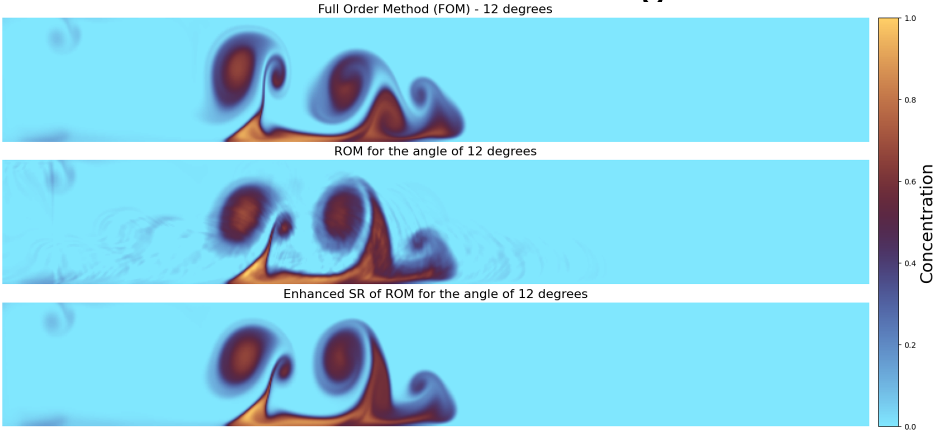
Comparison between a Finite Element Method data (top), Reduced order model data(middle), and the super-resolution enhanced data (bottom) at time 20s.

Error Analysis of the reconstruction - $\theta = 5$ degrees at 20s



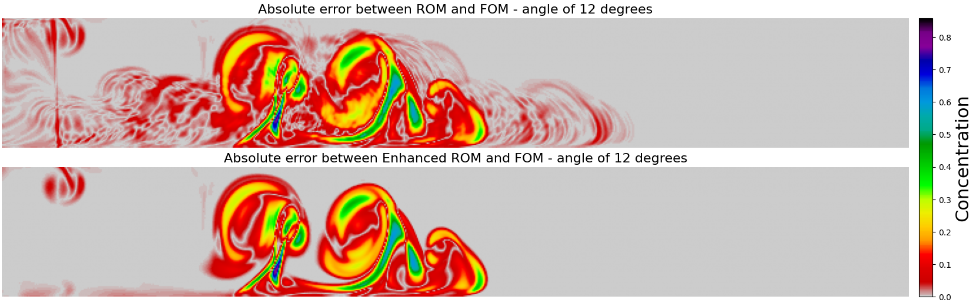
Comparison between the absolute error between the ROM and the FEM data (top) and between SR and FEM data (bottom) at time 20s.

Visual of the reconstruction - θ=12 degrees at 15s



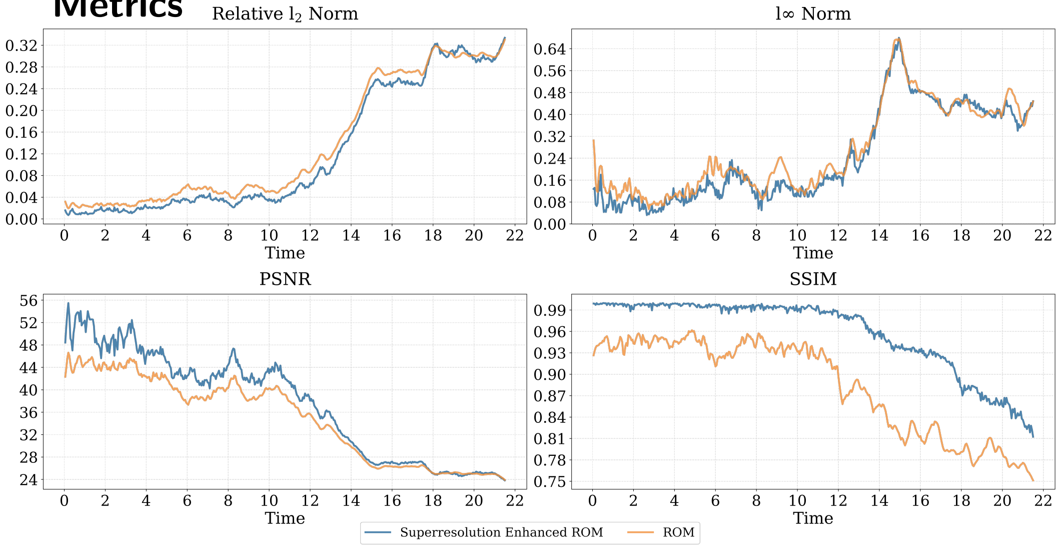
Comparison between a Finite Element Method data (top), Reduced order model data(middle), and the super-resolution enhanced data (bottom) at time 15s.

Error Analysis of the reconstruction - θ=12 degrees at 15s



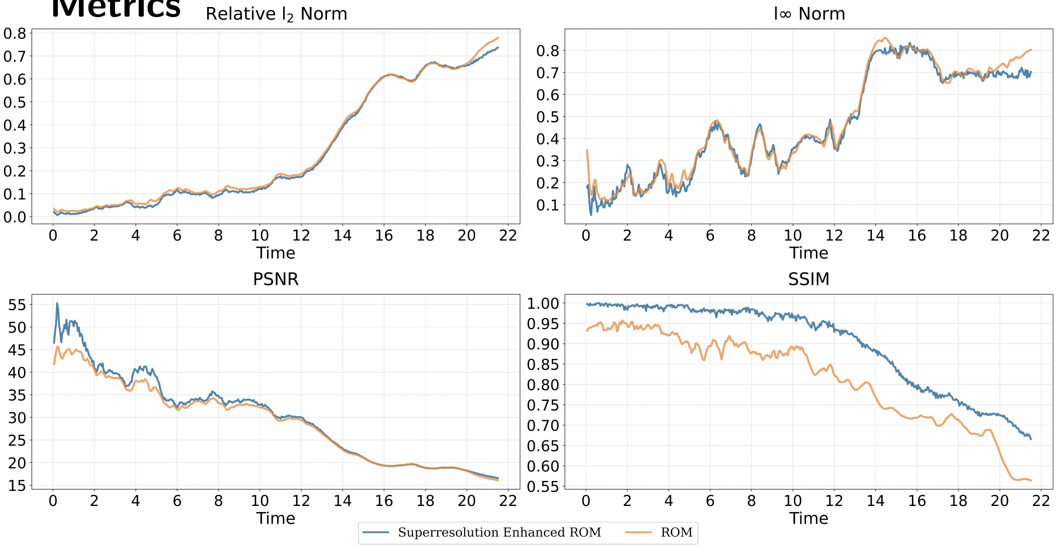
Comparison between the absolute error between the ROM and the FEM data (top) and between SR and FEM data (bottom) at time 15s.

Metrics



Metrics for the interpolation angle of 5 degrees.

Metrics



Metrics for the extrapolation angle of 12 degrees.

Conclusions

- S.R. model is able to increase fidelity of ROM, fixing numerical artifacts and reducing error;
- But increase in fidelity is limited by quantity of information in ROM, since the model is data-driven;
- Achieved robust image reconstruction in ROM reconstruction;
- Trainable with the same data used to build a surrogate.

[1] R. Sousa, R. Velho, N. Matos, A. Côrtes, G. Barros, A. Coutinho - **Data-driven diffusion-based super-resolution for improvement of reduced-order model predictions in fluid dynamics** - Preprint, 2025

Future Directions

- Experiment with alternative models, like Denoising Diffusion Restoration Models;
- Insert embedding (angle) in the diffusion model;
- Predictor for starting step of the reverse process;
- Effect of time splitting ROMS[1];
- Explore physics-informed guidance for improved fidelity.

[1] R. Velho, A. Côrtes, G. Barros, F. Rochinha. A. Coutinho - **Advances in Data-Driven Reduced Order Models using Two-Stage Dimension Reduction for Coupled Viscous Flow and Transport** - Preprint: https://papers.ssrn.com/sol3/papers.cfm?abstract_id=5064259 , 2024.

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Any question?

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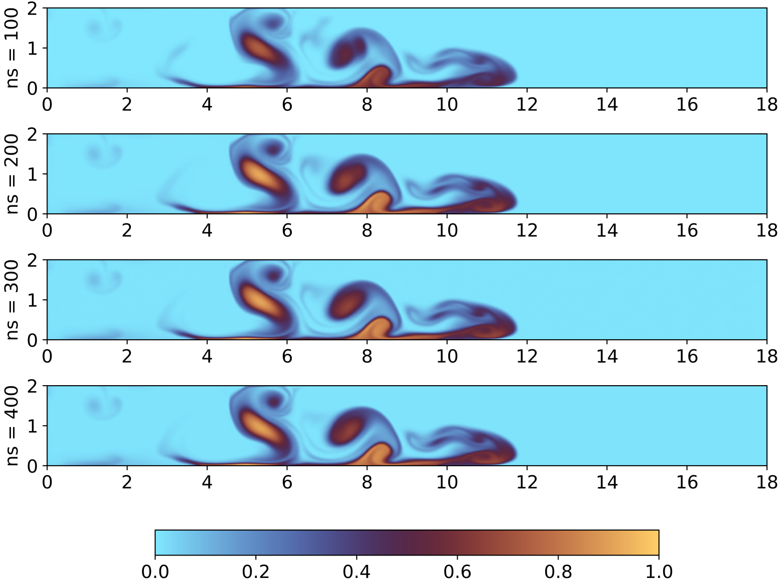
Slides, preprint, movies - https://github.com/rmvelho/cfc2025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