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► **To cite this version:**

Wilfried Genuist, Éric Savin, Filippo Gatti, Didier Clouteau. Data-driven Fluid Flow Prediction Using Conditional Score-based Diffusion Models. AICOMAS 2025 - Artificial Intelligence and computational Methodes in Applied sciences, Feb 2025, Paris, France. <hal-05120431>

HAL Id: hal-05120431

<https://hal.science/hal-05120431v1>

Submitted on 19 Jun 2025

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DATA-DRIVEN FLUID FLOW PREDICTION USING CONDITIONAL SCORE-BASED DIFFUSION MODELS

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Key Words: *Fluid mechanics, Diffusion models, Numerical simulations, PDEs*

ABSTRACT

Advances in computational power have made turbulent field simulations central to many disciplines, yet traditional solvers struggle to deliver fast flow estimations due to the inherent chaotic nature of the problem. More recently, diffusion models have set new benchmarks in generative modeling for similar problems. In this regard, we propose a data-driven conditional score-based diffusion model for transonic fluid flow prediction, integrating an energy constraint based on the flow statistics to enhance temporal stability.

Diffusion models aim at generating new samples from a dataset \mathcal{D} by inferring a score function (with optimization parameters θ) of a reverse time diffusion process. Additionally, we condition this process on the l previous states of the fluid flow [1] following an autoregressive formulation. By retrieving an estimated flow field $\hat{\mathbf{u}}_\theta$ from denoising score-matching (DSM) techniques [2], we can regularize the vanilla loss function \mathcal{L}_{DSM} by the random fluctuations of the fluid field through the autocorrelation matrix \mathbf{R} evaluated on times τ and $\tau - t_l$ (previous state of the fluid) and positions $\mathbf{r} \in \mathcal{R}$:

$$\mathcal{L}(\theta) = \mathcal{L}_{\text{DSM}}(\theta) + \mathbb{E}_{\substack{\mathbf{r}_1, \mathbf{r}_2 \in \mathcal{R} \\ \mathbf{u} \in \mathcal{D}}} \left\{ \left\| \mathbf{R}_{\mathbf{u}}(\mathbf{r}_1, \mathbf{r}_2, \tau - t_l, \tau) - \mathbf{R}_{\hat{\mathbf{u}}_\theta}(\mathbf{r}_1, \mathbf{r}_2, \tau - t_l, \tau) \right\|_2 \right\}.$$

Here \mathbb{E} stands for mathematical expectation, and \mathcal{L} is the regularized loss. The conditioning on the physical state is achieved using a denoising U-net architecture [3] combined with input concatenation, which has proven to be efficient in learning a conditional distribution.

Trained on a 2-dimensional transonic flow [1], inference is made on an extrapolation problem on Mach number in the set $\{0.50, 0.51, 0.52\}$ which is notoriously hard to predict as shock waves occur frequently (compared to the training set).

Early results¹ (**Fig. 1.**) demonstrate that incorporating an energy loss function has been crucial in maintaining temporal stability and coherence in the intermediate predictions, however, achieving accurate results over longer time horizons (Lyapunov time $\tau_{Ly} > 15$) remains challenging.

¹ Animated results are available on: <https://nextcloud.centralesupelec.fr/s/3zj7eTfcsCoTmtA> and <https://nextcloud.centralesupelec.fr/s/e6KdYRwGQHjFaSL>.

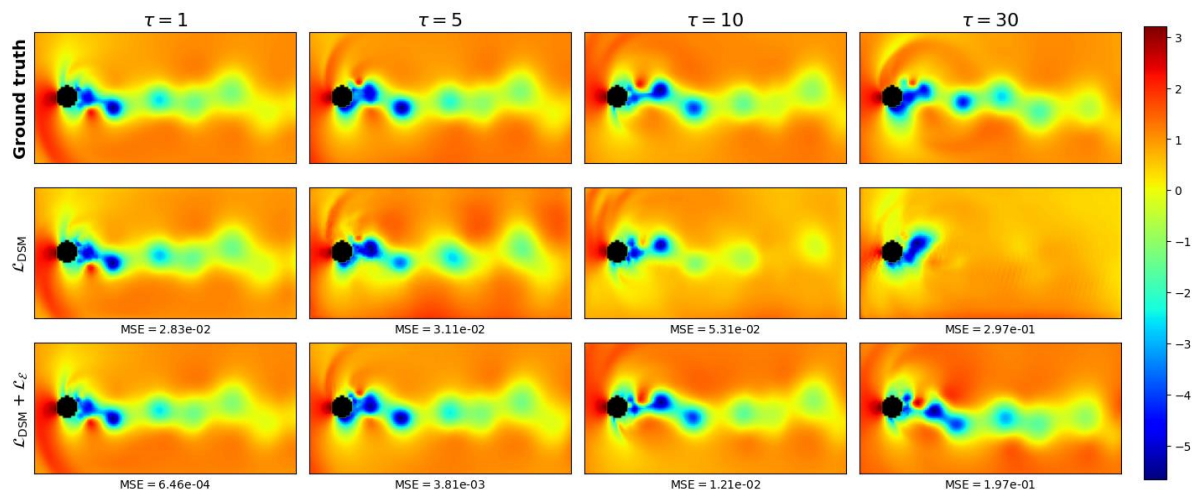


Fig. 1. Prediction of the pressure field at Mach 0.5.

While the autoregressive formulation hinders sampling time, diffusion models have demonstrated strong extrapolation capabilities. Transitioning to latent space presents a promising avenue for further improvement.

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