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Uncertainty Quantification for GPU-Accelerated High-Fidelity DNS Investigation of Supersonic Retro Propulsion (SRP) Flow During Martian Descent Using High-Order Flux Reconstruction in PyFR using Surrogate Modelling (Machine Learning approach): An approach to advance sustainable space exploration

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PyFR

Introduction:

Supersonic retro-propulsion has emerged as a key technology for controlled planetary descent, particularly for high-mass payload landings on Mars. The interaction between high-speed retrograde jets and the supersonic freestream results in complex aerodynamic phenomena, including bow shocks, shear layer instabilities, and recirculation zones. Understanding these interactions is crucial for designing efficient descent systems.

Traditional computational fluid dynamics (CFD) methods often struggle to resolve these flow features due to high computational costs. This study employs a DNS approach using PyFR, an open-source high-order solver based on the flux reconstruction method, to achieve greater accuracy. The use of GPU acceleration significantly improves computational efficiency, making high-fidelity SRP simulations feasible while supporting sustainable engineering practices in aerospace design.

Co-kriging Data fusion and Adaptive sampling technique has been used to obtain the precise data predictions for the lift and drag within the confined domain without conducting the costly simulations on HPC clusters. This creates a methodology to quantifying uncertainty in computational fluid dynamics by minimizing the required number of samples. To minimize the reliability on high-fidelity numerical simulations in Uncertainty Quantification, a multi-fidelity strategy has been adopted [1,3].

Abstract:

The first stage of research presents a high-fidelity direct numerical simulation (DNS) of supersonic retro-propulsion (SRP) flow during Martian descent using the high-order flux reconstruction method in PyFR. The research aims to improve the understanding of complex flow structures, shock interactions, and aerodynamic effects induced by SRP while leveraging GPU acceleration for computational efficiency. The insights gained contribute to optimizing fuel usage, reducing mission risks, and enhancing the sustainability of future Mars landing systems. The findings are relevant for developing reusable descent architectures, improving computational resource efficiency, and supporting long-term space exploration sustainability [2]. The later part of the research involves extracting Coefficient of lift and Coefficient of drag data for Reduced Order modelling. Co-kriging Data fusion and adaptive sampling technique has been used to obtain the precise data predictions for the lift and drag within the confined domain without conducting the costly simulations on HPC clusters. This creates a methodology to quantifying uncertainty in computational fluid dynamics by minimizing the required number of samples. In order to minimize the reliability on high-fidelity numerical simulations in Uncertainty Quantification, Machine learning strategy has been adopted, and the effectiveness of the Machine learning model has been validated through the approximation of benchmark function tests (both linear and nonlinear correlations) [1,3]

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Methodology:

The study utilizes PyFR to conduct DNS of SRP flowfields, leveraging high-order flux reconstruction on unstructured meshes for accurate turbulence and shockwave resolution. The key simulation parameters include:

- **Flow Regime:** Supersonic freestream with retro-propulsion jet interaction
- **Numerical Scheme:** High-order flux reconstruction on unstructured grids
- **Computational Resources:** Multi-GPU architecture for parallel processing
- **Validation Approach:** Comparison with available experimental and computational datasets

A structured workflow is implemented, including mesh generation, numerical setup, and post-processing to analyze key flow structures such as jet-induced recirculation, shock-shock interactions, and turbulence characteristics.

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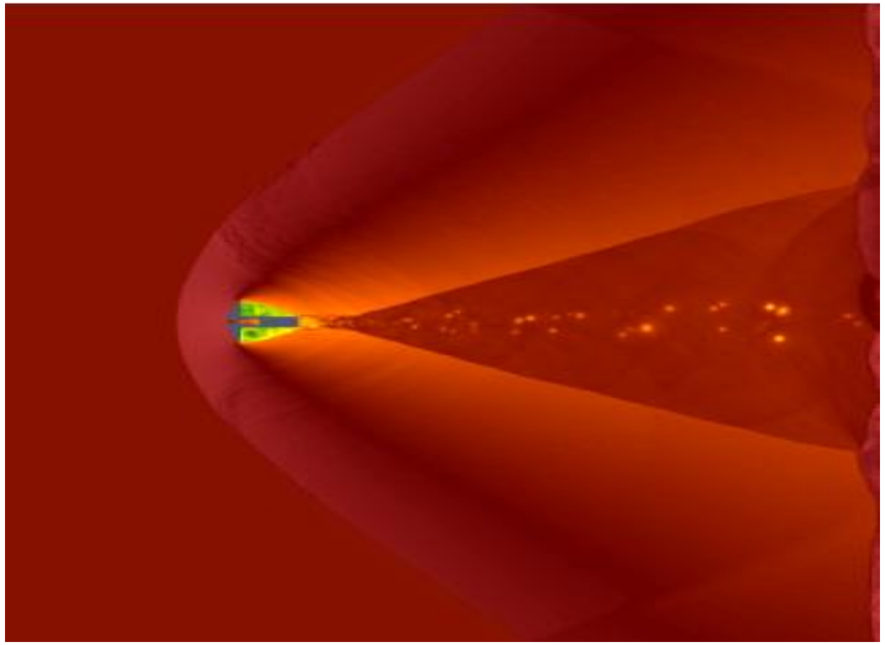

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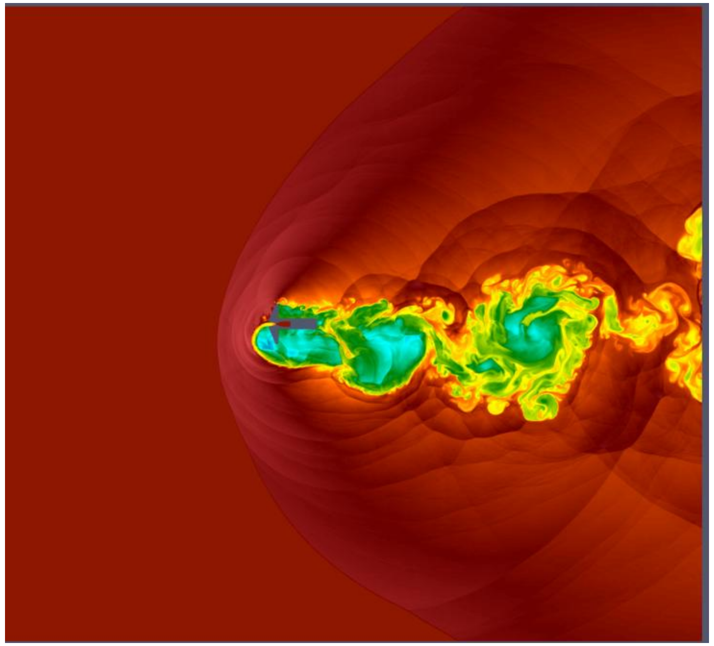

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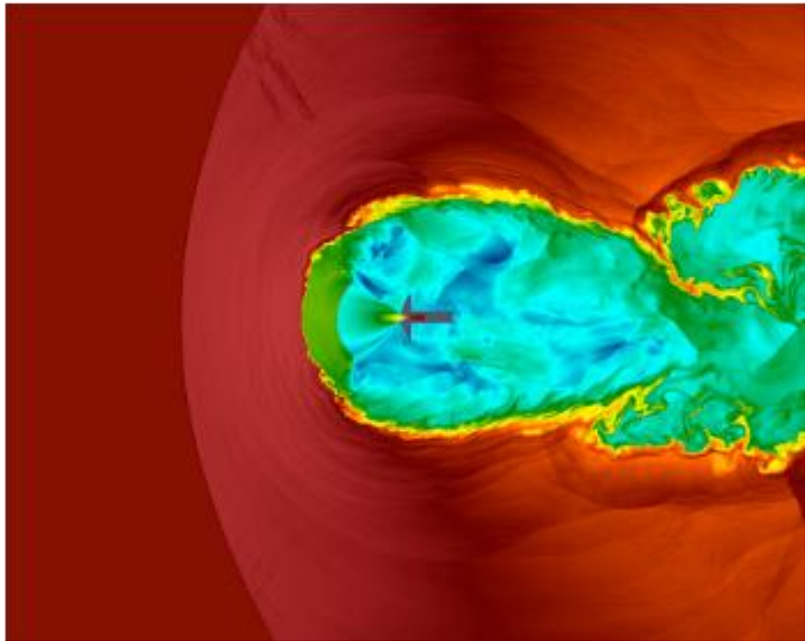

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Short Penetration Mode: Stable Mode

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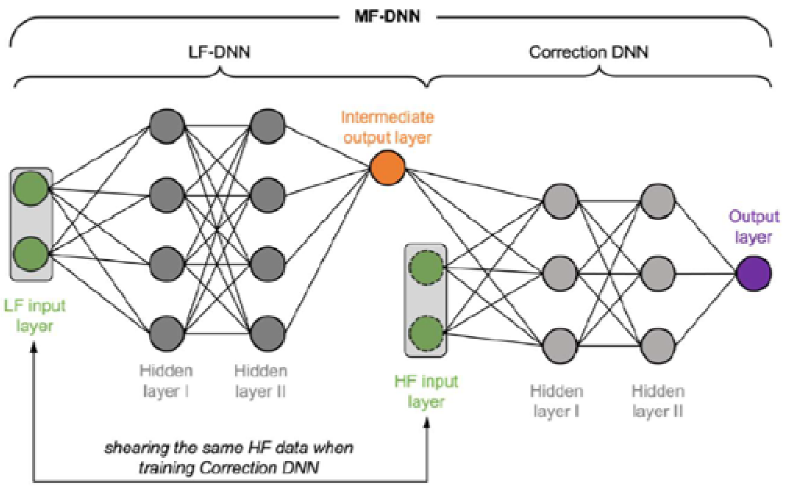

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Function 1

$$y_L(x) = 0.5y_H + 10(x - 0.5) - 5$$

$$y_H(x) = (6x - 2)^2 \sin(12x - 4)$$

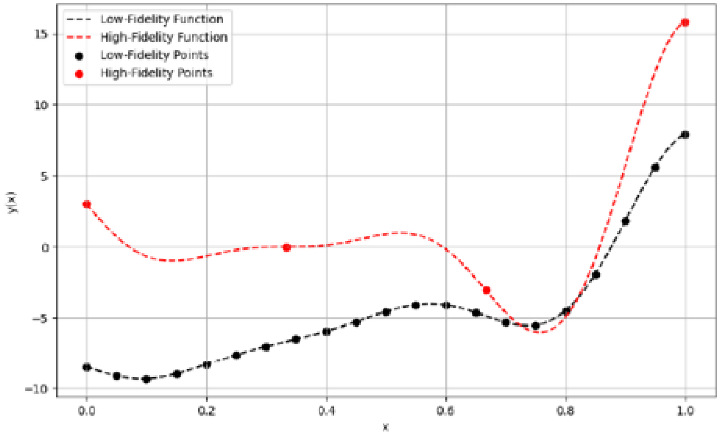

Table 3.2: Mean Square Error (MSE) prediction for function benchmark test

Model	MSE Value
MF-DNN ReLU	9.73e-03
RBF	28.5204e+00
Co-Kriging	4.77336e-09

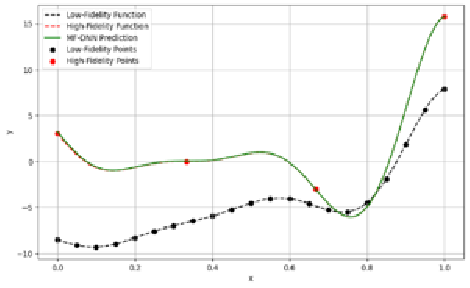

Figure 3.9: MF-DNN in approximating 1-dimension function

Function 2

$$y_L(x) = 0.5(6x - 2)^2 \sin(12x - 4) + 10(x - 0.5) - 5$$

$$y_H(x) = 0.1y_L(x)^2 + 10$$

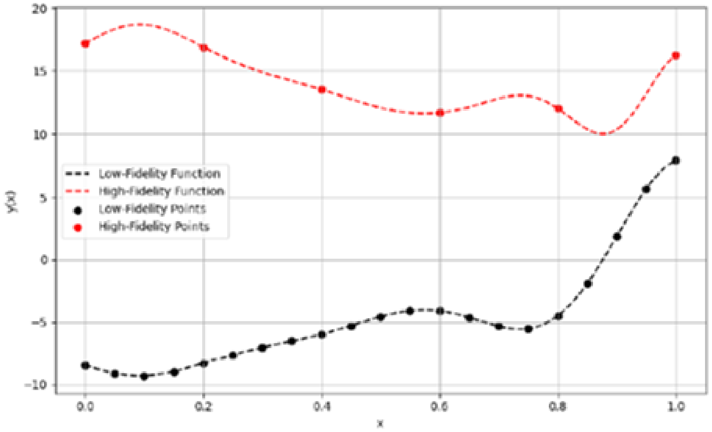

Table 3.3: Mean Square Error (MSE) prediction for the function benchmark test

Model	MSE Value
MF-DNN ReLU	1.17e-02
RBF	1.4876e+00
Co-Kriging	4.4034435e+00

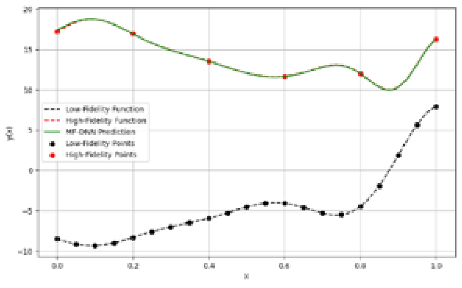

Figure 3.10: MF-DNN in approximating 1-dimension function

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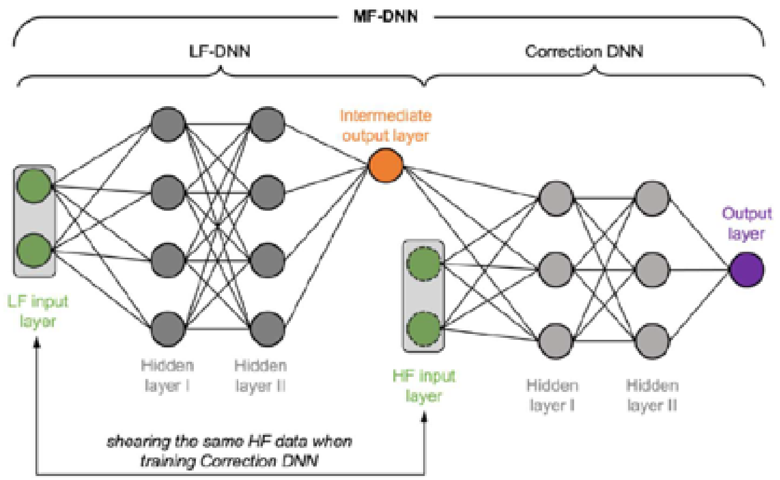

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Function 1-D

$$y_L(x) = 0.5y_H + 10(x - 0.5) - 5$$

$$y_H(x) = (6x - 2)^2 \sin(12x - 4)$$

Function 1-D

$$y_L(x) = 0.5(6x - 2)^2 \sin(12x - 4) + 10(x - 0.5) - 5$$

$$y_H(x) = 0.1y_L(x)^2 + 10$$

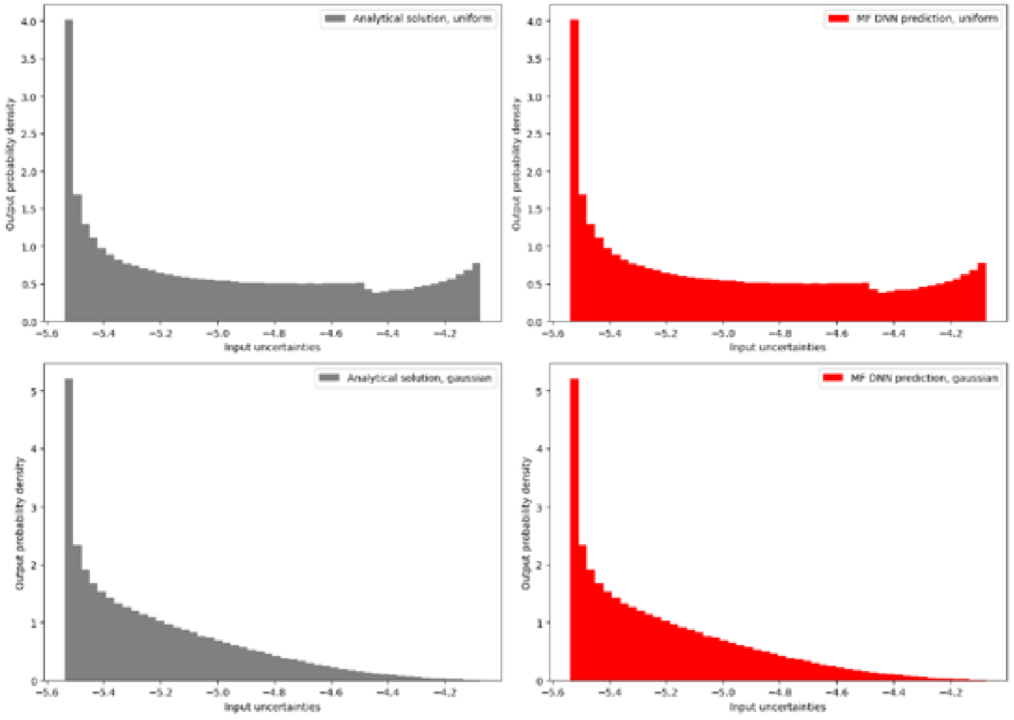
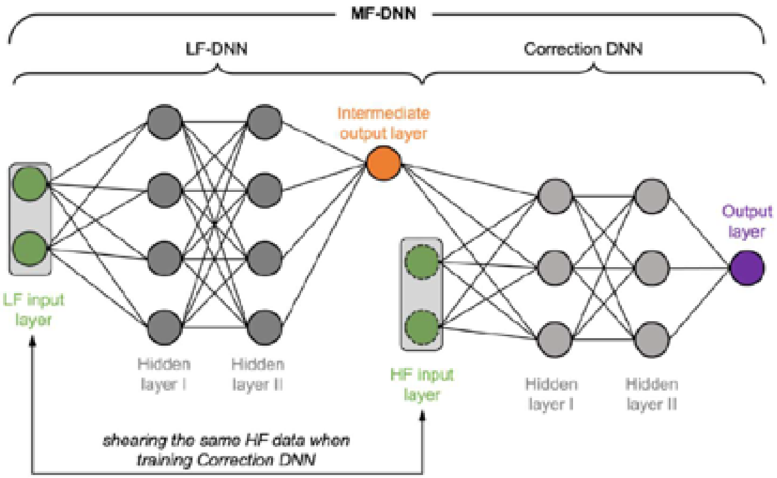


Figure 3.13: Histogram comparison of QoI probability density distribution, 1-dimension function

32-D function

$$y_L(x_0, \ldots, x_{31}) = 0.8 \times y_H - 0.4 \sum_{i=0}^{30} (x_i x_{i+1}) - 50, \quad x_i \in [-3, 3]$$

$$y_H(x_0, \ldots, x_{31}) = (x_0 - 1)^2 + \sum_{i=1}^{31} (2x_i^2 - x_{i-1}^2)^2, \quad x_i \in [-3, 3]$$



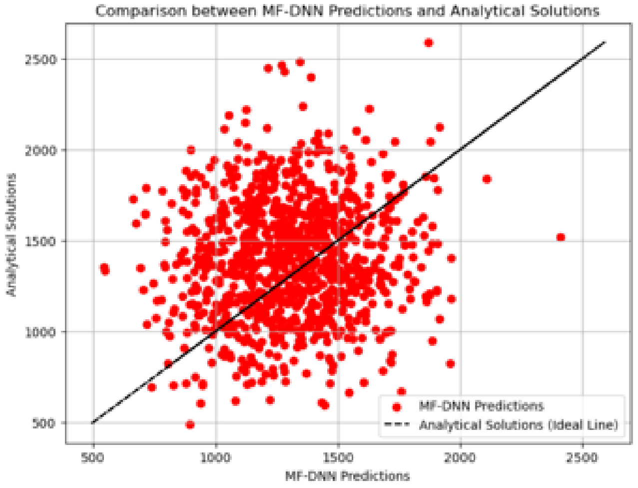


Figure 3.11: MF-DNN in approximating 32-dimensional function

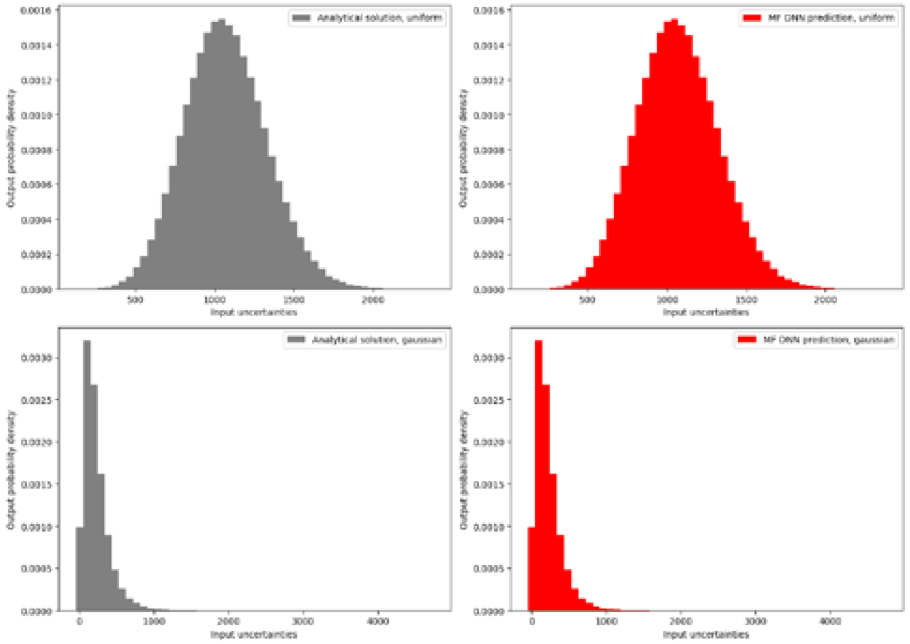


Figure 3.14: Histogram comparison of QoI probability density distribution, 32-dimensional function

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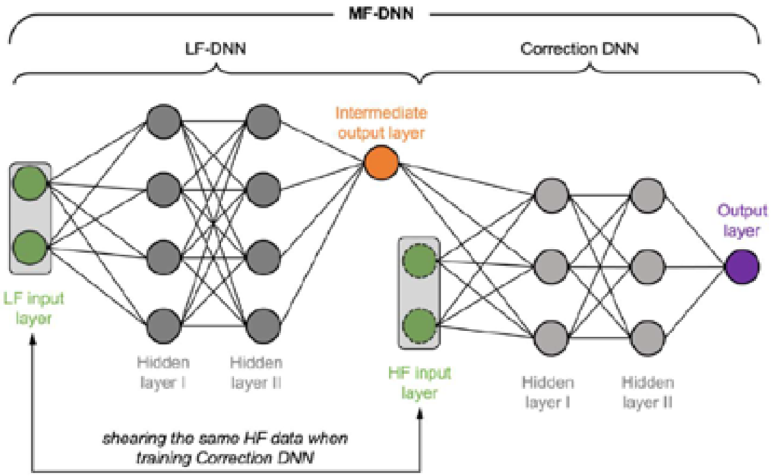
100-D function

$$y_L(x_0,\dots,x_{99}) = 0.8\times y_H - 0.4\sum_{i=0}^{98}(x_i x_{i+1}) - 50, \quad x_i\in[-3,3]$$

$$y_H(x_0,\dots,x_{99}) = (x_0-1)^2 + \sum_{i=1}^{99}(2x_i^2 - x_{i-1}^2)^2, \quad x_i\in[-3,3]$$



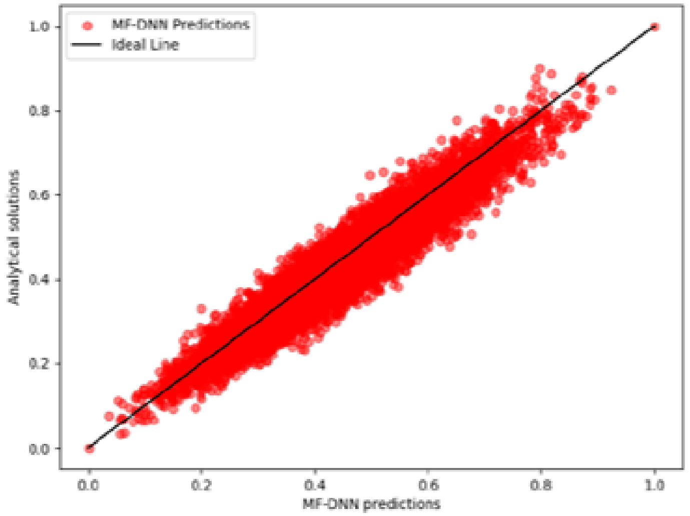


Figure 3.12: Performance of MF-DNN model for 100-dimensional function

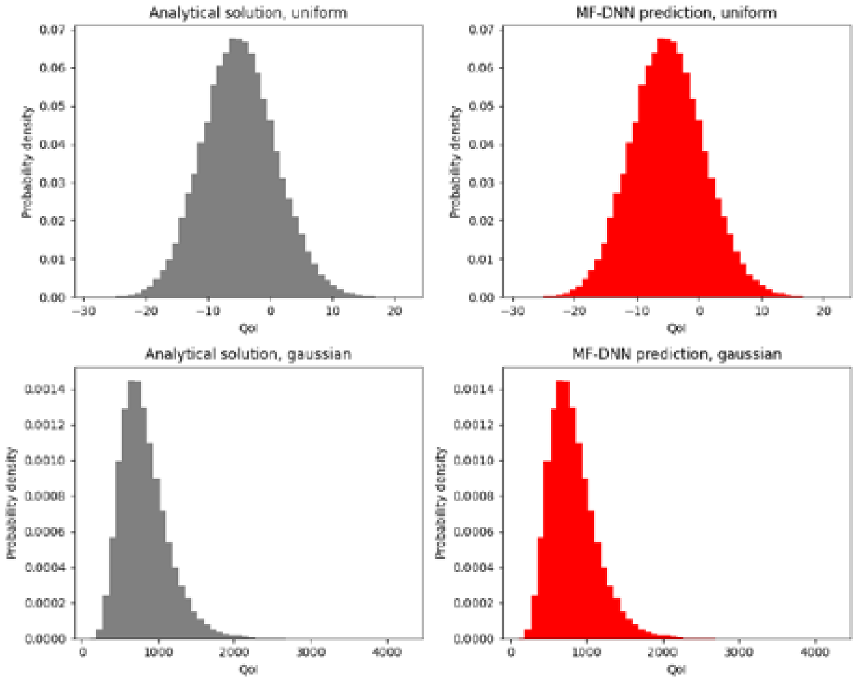


Figure 3.15: Histogram comparison of QoI probability density distribution, 100-dimensional function

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Conclusions:

- This research demonstrates the feasibility and benefits of GPU-accelerated DNS for investigating SRP flows during Martian descent. The use of high-order flux reconstruction in PyFR provides detailed insights into shock interactions and turbulence dynamics, contributing to safer, more efficient, and sustainable planetary landings. The work supports sustainable space exploration by optimizing fuel efficiency, improving reusability, and reducing computational waste. Future research will focus on expanding the parameter space, further optimizing computational efficiency, and refining turbulence modeling approaches to enhance SRP technology for Mars and beyond [2].
- Co-kriging Data fusion and Adaptive sampling technique has been used to obtain the precise data predictions for the lift and drag within the confined domain without conducting the costly simulations on HPC clusters. This creates a methodology to quantifying uncertainty in computational fluid dynamics by minimizing the required number of samples. To minimize the reliability on high-fidelity numerical simulations in Uncertainty Quantification, a multi-fidelity strategy has been adopted. The effectiveness of the multi-fidelity deep neural network model has been validated through the approximation of benchmark functions across 1-, 32-, and 100-dimensional, encompassing both linear and nonlinear correlations [1,3].

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Conclusions:

- The surrogate modelling results showed that multi-fidelity deep neural network model has shown excellent approximation capabilities for the test functions and multi-fidelity deep neural network method has outperformed Co-kriging in effectiveness [1,3].

- In addition to that, multi-fidelity deep neural network model is utilized for the simulation of aleatory uncertainty propagation in 1-, 32-, and 100-dimensional function test, considering both uniform and Gaussian distributions for input uncertainties [1,3].

- The results have shown that multi-fidelity deep neural network model has efficiently predicted the probability density distributions of quantities of interest as well as the statistical moments with precision and accuracy [1,3].

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1. Swapnil Kumar, Francesco Montomoli, Uncertainty Quantification for Multi-Fidelity Simulations (Scientific Machine Learning & Uncertainty Quantification), Imperial College London, 2024, https://www.researchgate.net/publication/380369138_Uncertainty_Quantification_for_Multi-Fidelity_Simulations_Scientific_Machine_Learning_Uncertainty_Quantification

2. Debdoot Ghosh, Peter Vincent, GPU-Accelerated High-Fidelity DNS Investigation of Supersonic Retro Propulsion (SRP) Flow During Martian Descent Using High-Order Flux Reconstruction in PyFR, Imperial College London, 2024.

3. Zhihui Li, Francesco Montomoli, Aleatory uncertainty quantification based on multi-fidelity deep neural networks, Reliability Engineering & System Safety, Volume 245, 2024,109975, ISSN 0951-8320, https://doi.org/10.1016/j.ress.2024.109975. (https://www.sciencedirect.com/science/article/pii/S0951832024000504)