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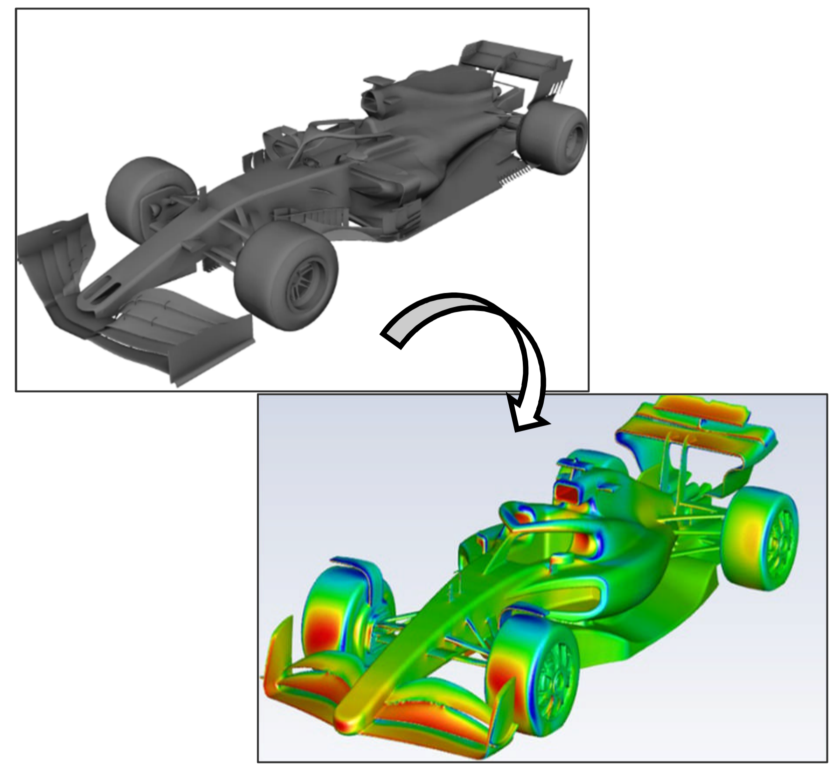
An Advanced Surrogate Model Approach for Enhancing Fluid Dynamics Simulations



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Motivation

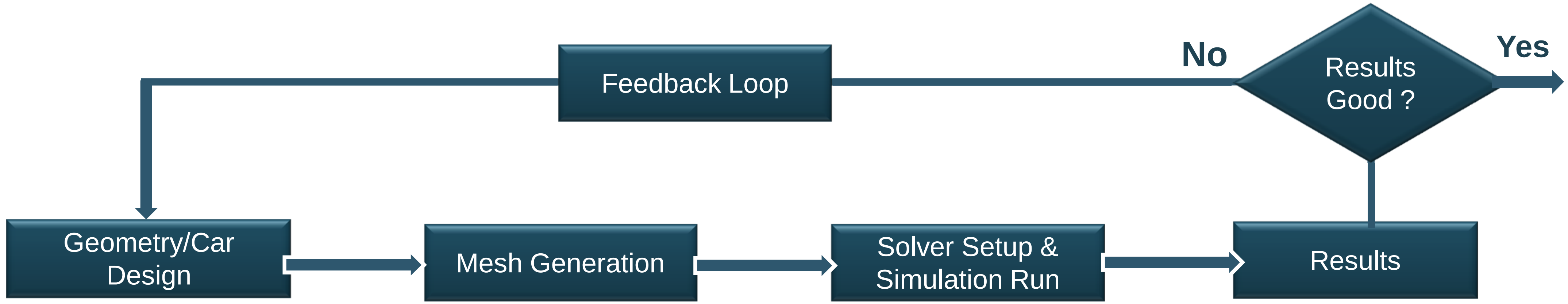
Motivation

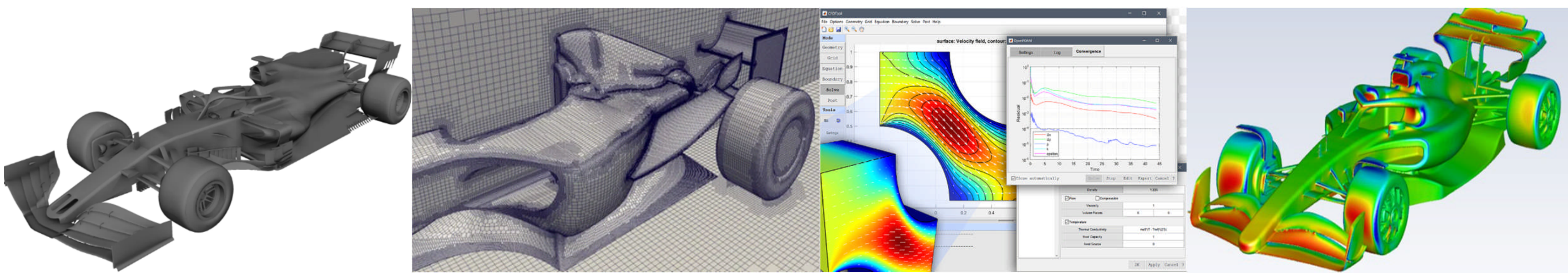
Challenges with Traditional Fluid Dynamic Simulations

- **Objective:** Design a car shape that minimizes drag and enhances fuel efficiency**.**

  - Currently, **Computational Fluid Dynamics (CFD)** methods are used for simulations
  - These methods provide **high accuracy but are slow.**
  - **Restricts** their use in **rapid design iterations** during the optimization process.

Traditional CFD method Pipeline



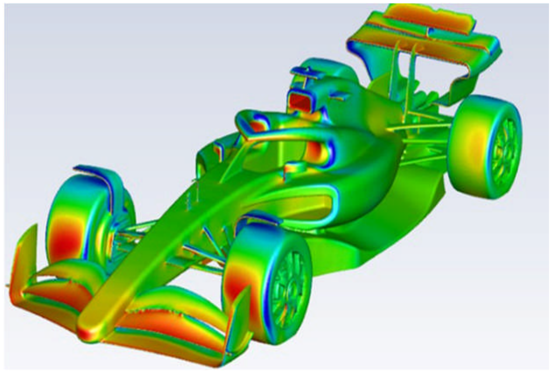


Why Deep Learning (DL) based Surrogate Models?

- Surrogate models offer **faster predictions**
- They enable **quick design iterations**, accelerating the path to an optimized solution

Aim: To develop an efficient surrogate model for accurate prediction of fluid flows

Input to Model



Final Results from Model

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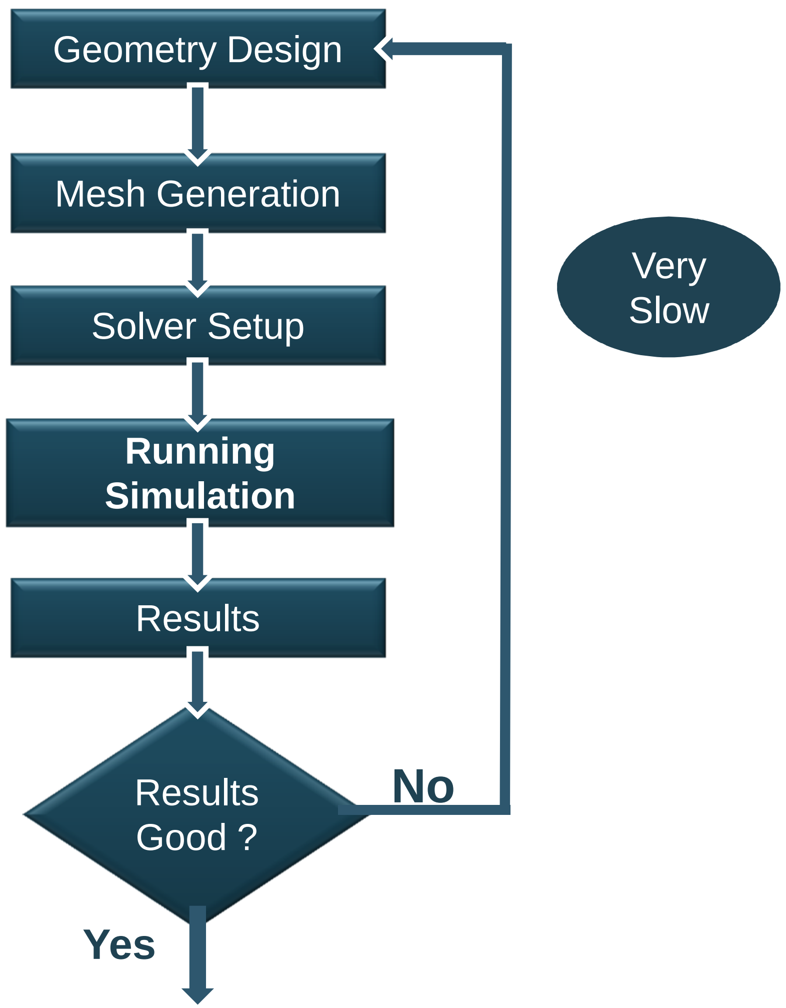
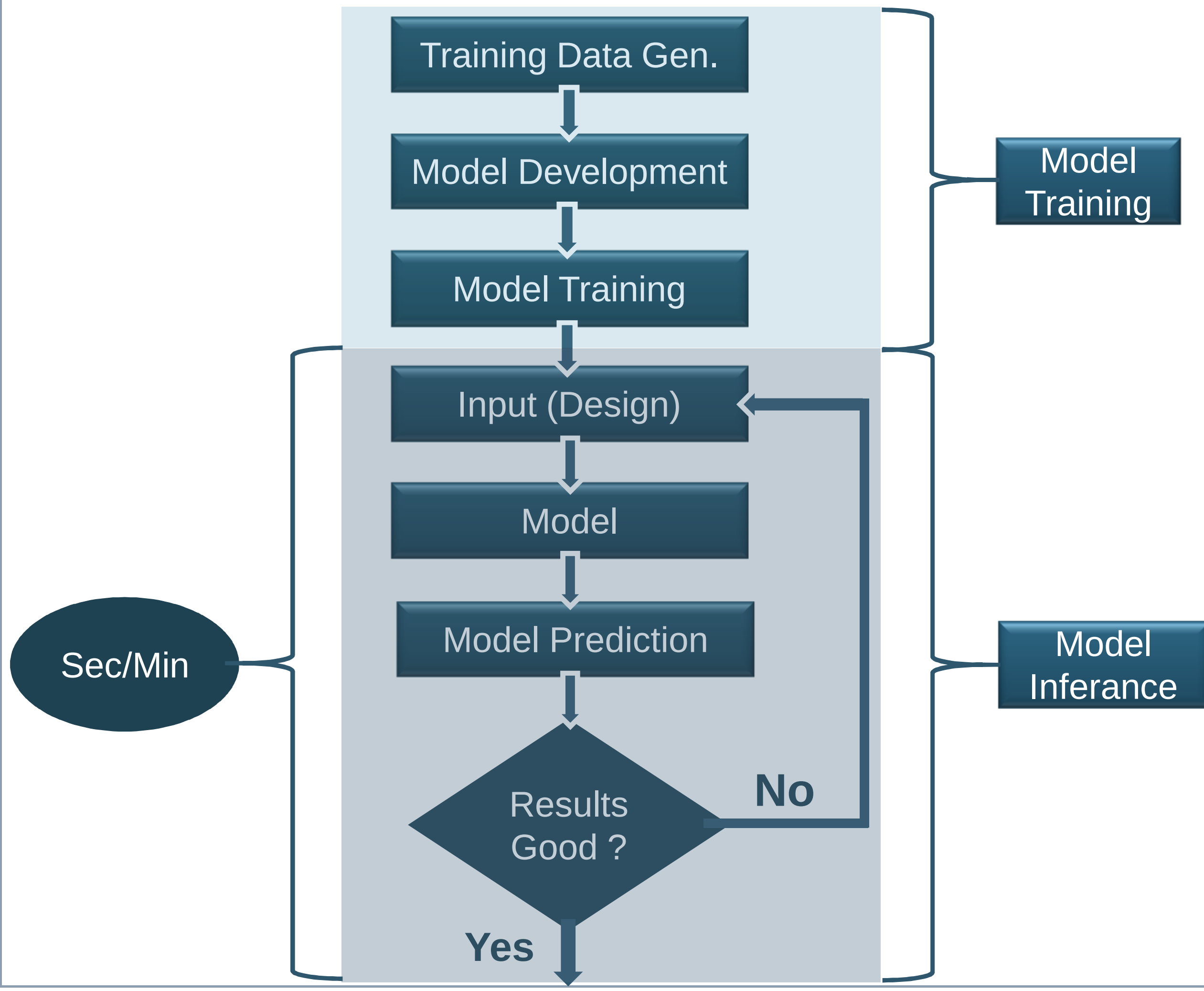
Pipeline : Traditional CFD Vs Surrogate Model

Pipeline - Traditional CFD



Pipeline – Surrogate Model



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Development of Surrogate Model

Training Data

- **Channel Flow** is considered to generate the training data
- **3-D Primitive geometries** are randomly created to obstruct the fluid flow

- The **Lattice Boltzmann Method (LBM)** -based framework, **waLBerla**, is utilized for simulations
- The **D3Q27** model with **periodic boundary conditions** is used to generate true labels

- **Signed Distance Fields (SDF)** are used to represent the object's shape and surrounding fluid field

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Deep Learning Model for Fluid Predictions

- **U-Net architecture** is employed for **flow prediction**
- Initially, a standard U-Net model was developed
- **Results** from the standard U-Net indicated the **need for architectural improvements**
- Building on these insights, an **advanced U-Net model was developed to enhance performance**

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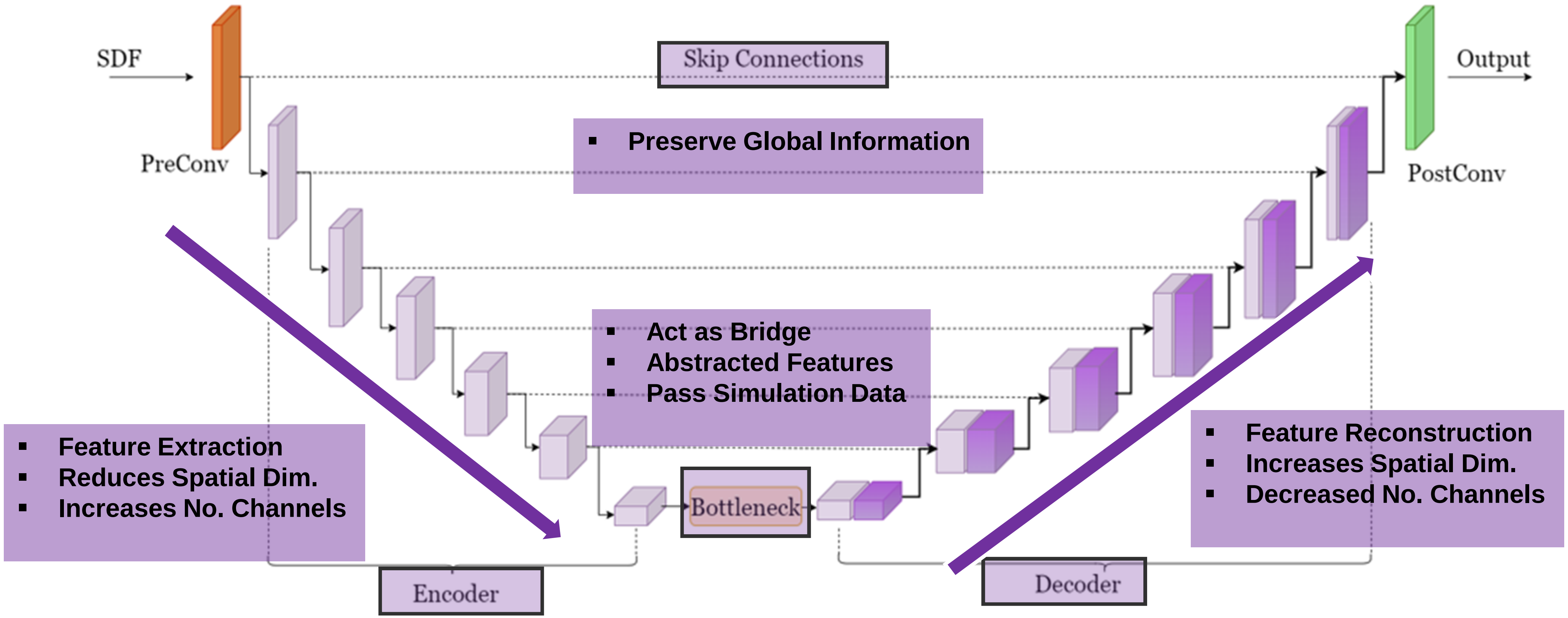
Understanding Standard U-Net Architecture

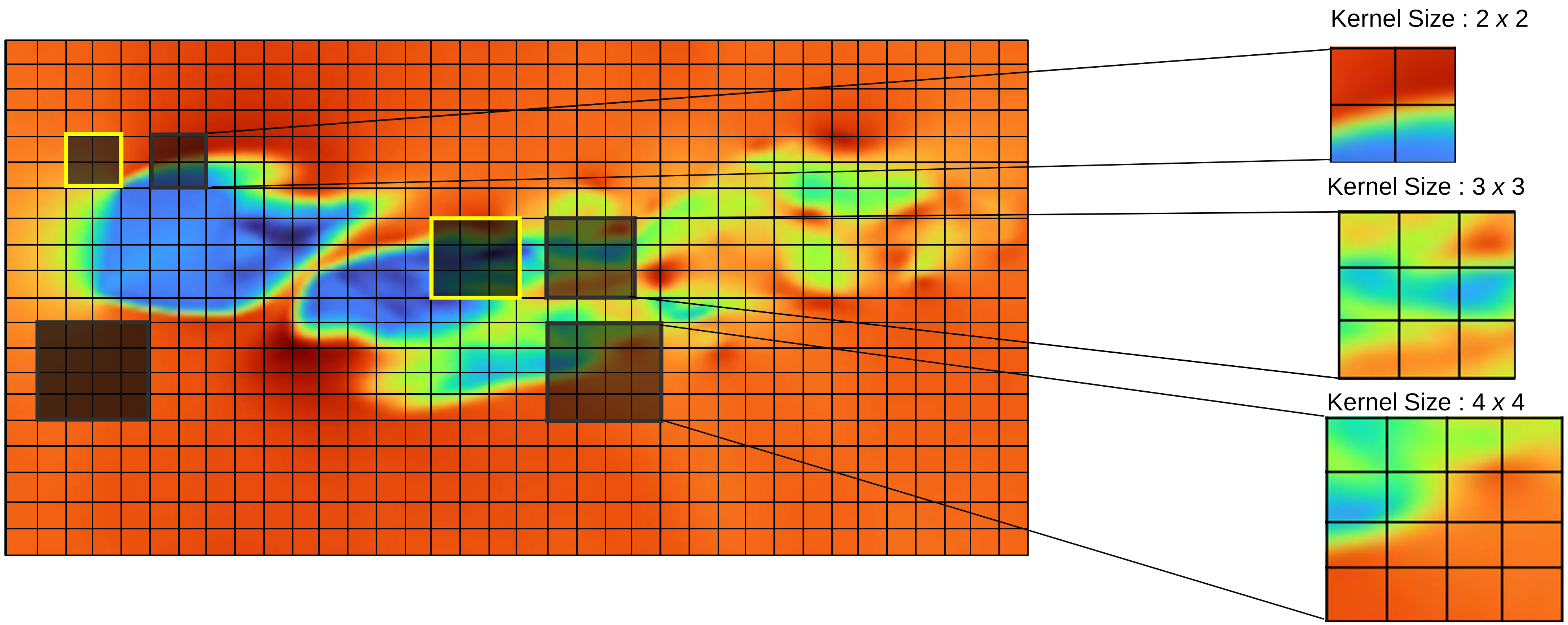


Standard U-Net Architecture

Advanced U-Net Architecture: Key Enhancement

Different Kernel Sizes

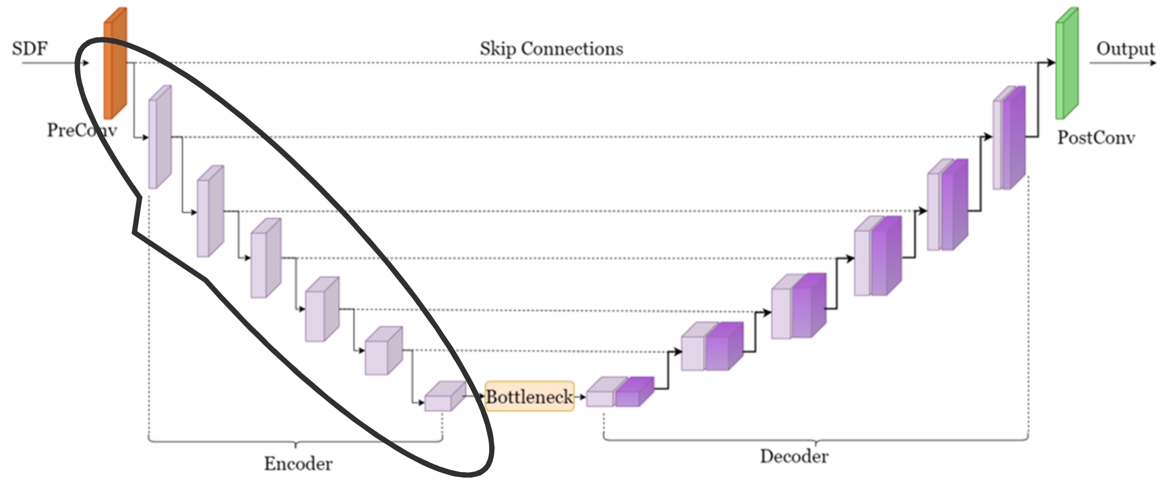
- ❑ Allows the network to focus on **features at different scales**

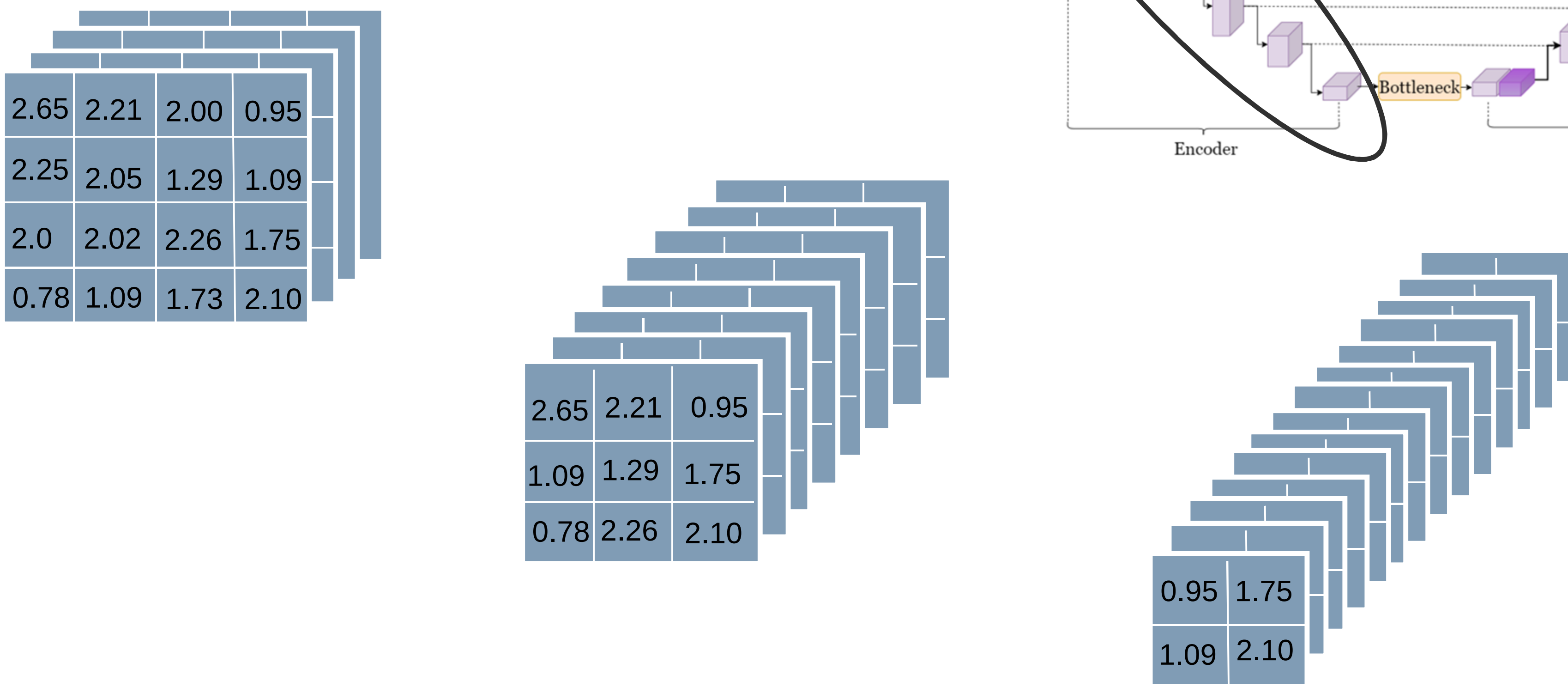


Advanced U- Net Architecture: Key Enhancement

Increased encoder layers and number of channels (up to 4096).

- ❑ **Learned Features** are stored in **channels**
- ❑ **Gradual decrease** of spatial dimensions is important to **preserve fine-details**

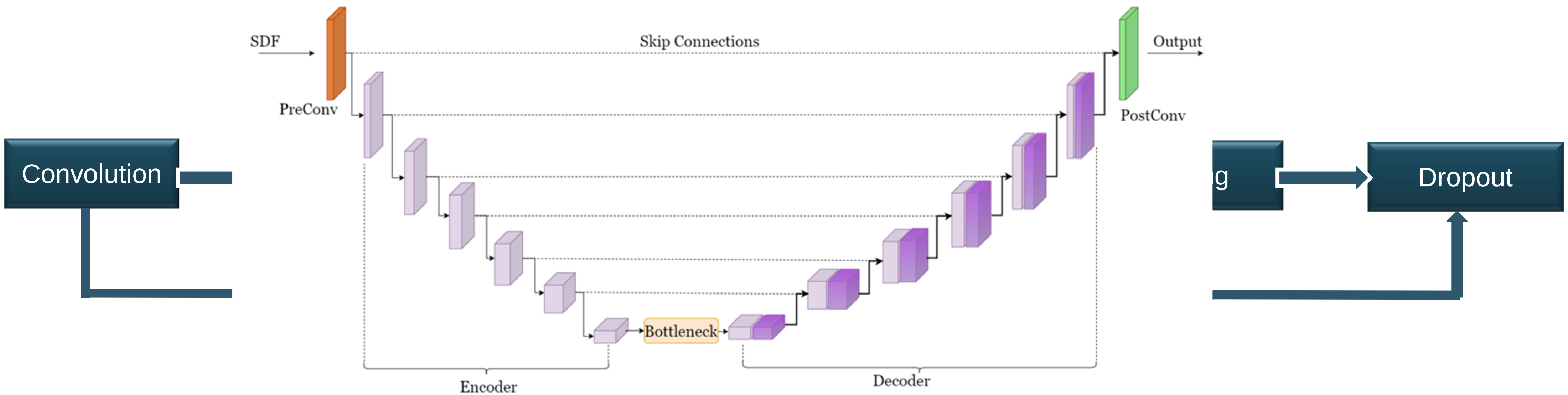




Advanced U- Net Architecture: Key Enhancement

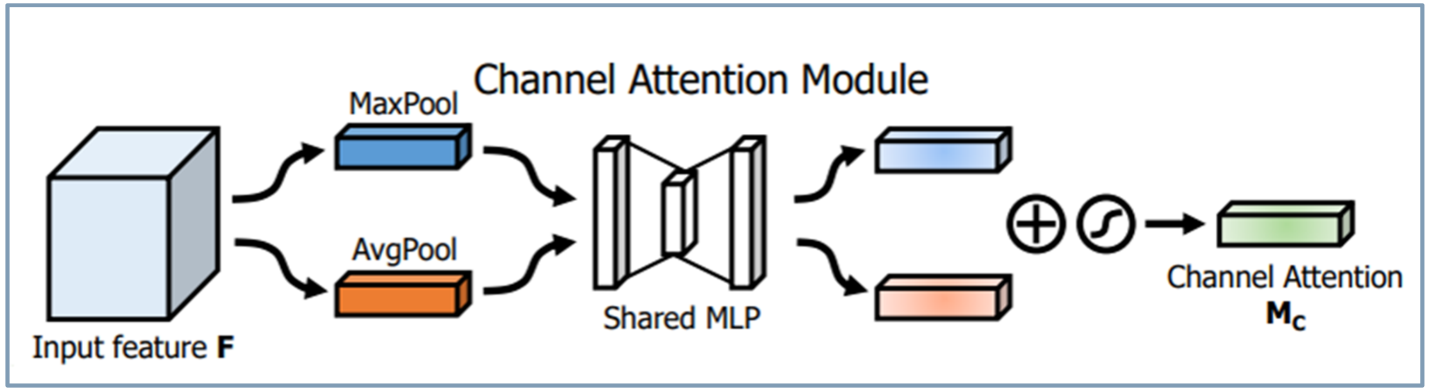
Skip Connections Inside Encoder and Decoder Block.

- ❑ Operations with Potential Information Loss

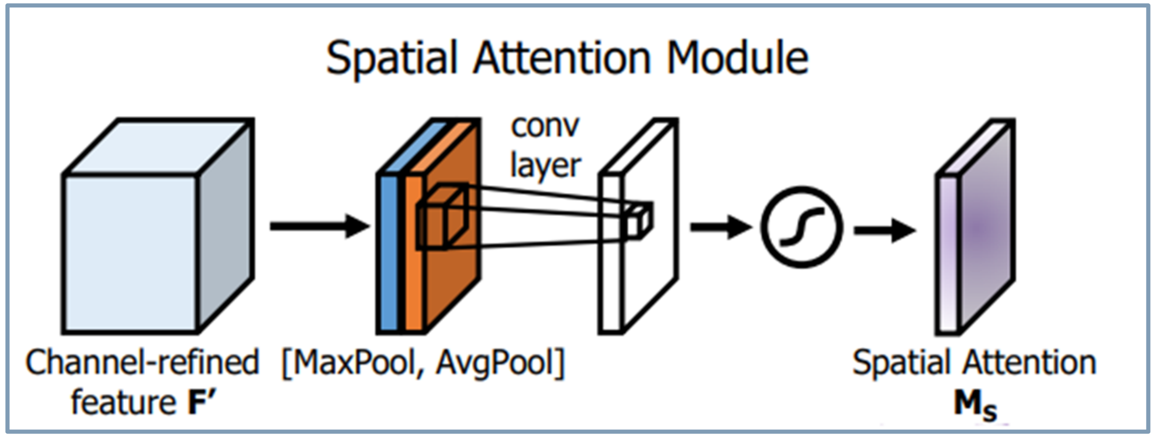


Advanced U- Net Architecture: Key Enhancement

Convolution Block Attention Module (CBAM)



Focus : Which
Which Features Imp. ?



Focus : Where ?
Features Location

Comparing Standard U-Net and Advanced U-Net

Feature	Standard Model	Advanced Model
Number of Encoder Layers	6	11
Number of Decoder Layers	6	11
Total Number of Channels	512	4096
Attention Mechanism	✗	Convolution Block Attention Module (CBAM)
Increased No. of Encoder Layers	✗	✓
Use of Skip Connection in Encoder and Decoder Block	✗	✓

Comparison between Base model and Advanced U-net Model

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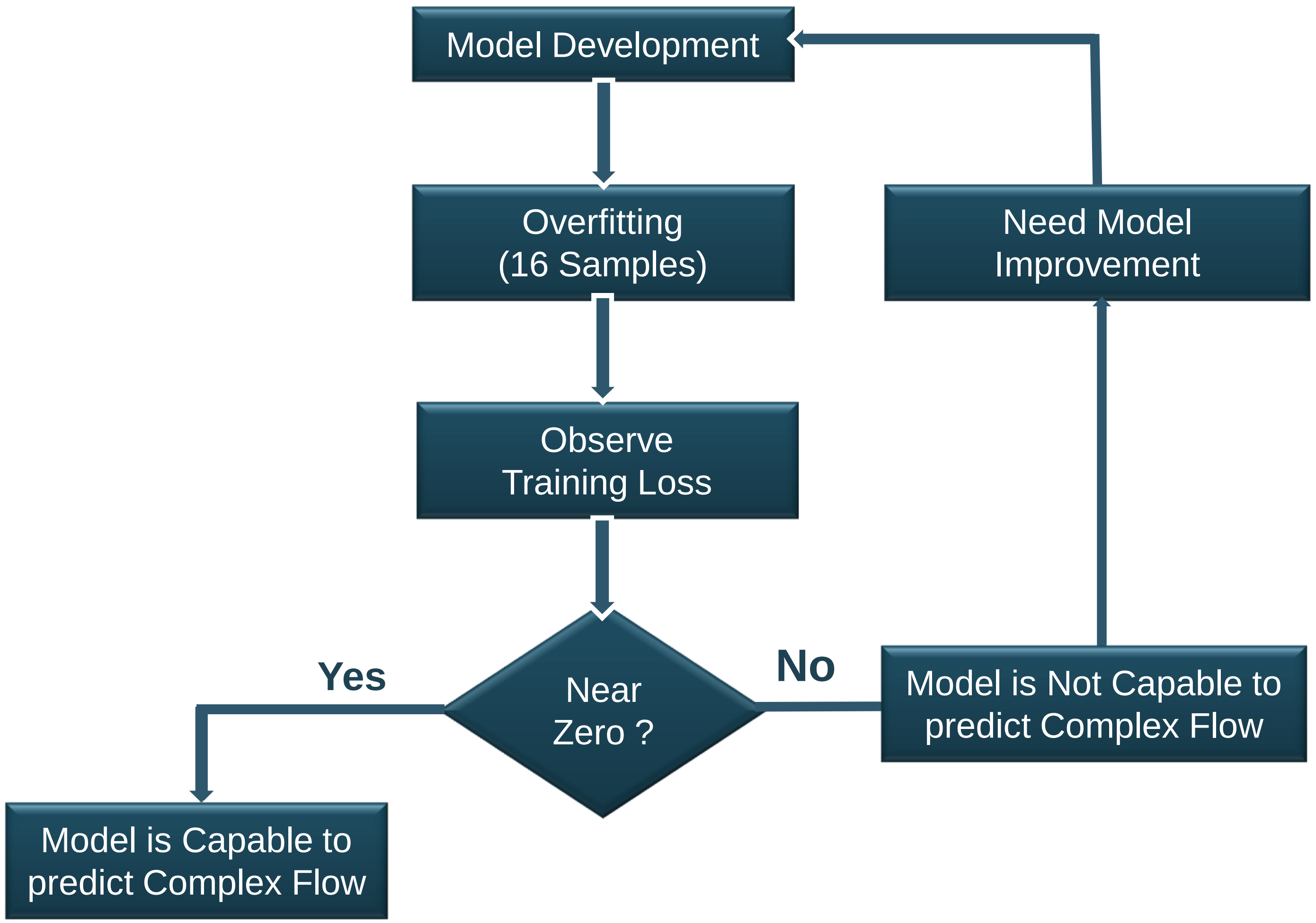
Training Methodology

Model Training Methodology

Model Capacity Evaluation through Overfitting



Model Training Methodology

Multi-GPU Training

- Trainable parameters increased from **46 million** in standard U-Net to **511 million** in Advanced U-Net
- Unable to fit the Advanced U-Net model into **single GPU memory**
- **Multi-GPU** setup is utilized for training
- **Data parallelism** was implemented using **PyTorch DDP**
- **Model parallelism** was implemented using **Deep Speed ZeRO-3**
- Training was conducted on **total 8, A100 GPUs.**

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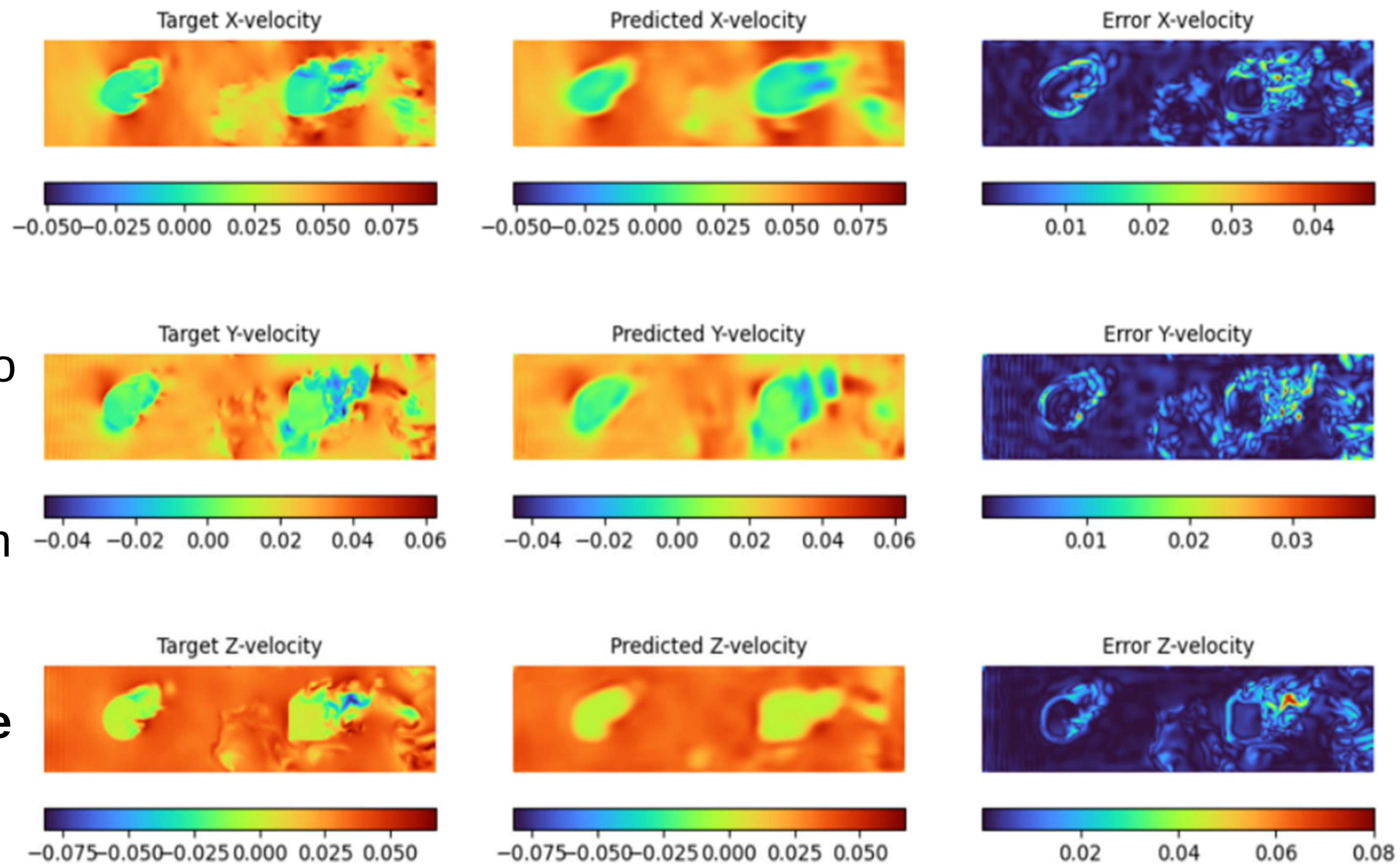
Initial Results

Results and Analysis : Standard U-Net Model

Model Capacity Evaluation through Overfitting

- ❑ Model is trained for **5000 epochs** using **16 training samples**
- ❑ **L1 loss of 0.32** was observed, far from the ideal loss of zero
- ❑ **Standard U-Net** model struggles to approximate the flow field.
- ❑ **Discrepancy** in prediction between different velocity components
- ❑ Suggests that the **model lacks the necessary capacity** for precise flow pattern prediction.



Comparison of Target Velocity, Predicted Velocity, and Absolute Error for Each Component for 16 data size

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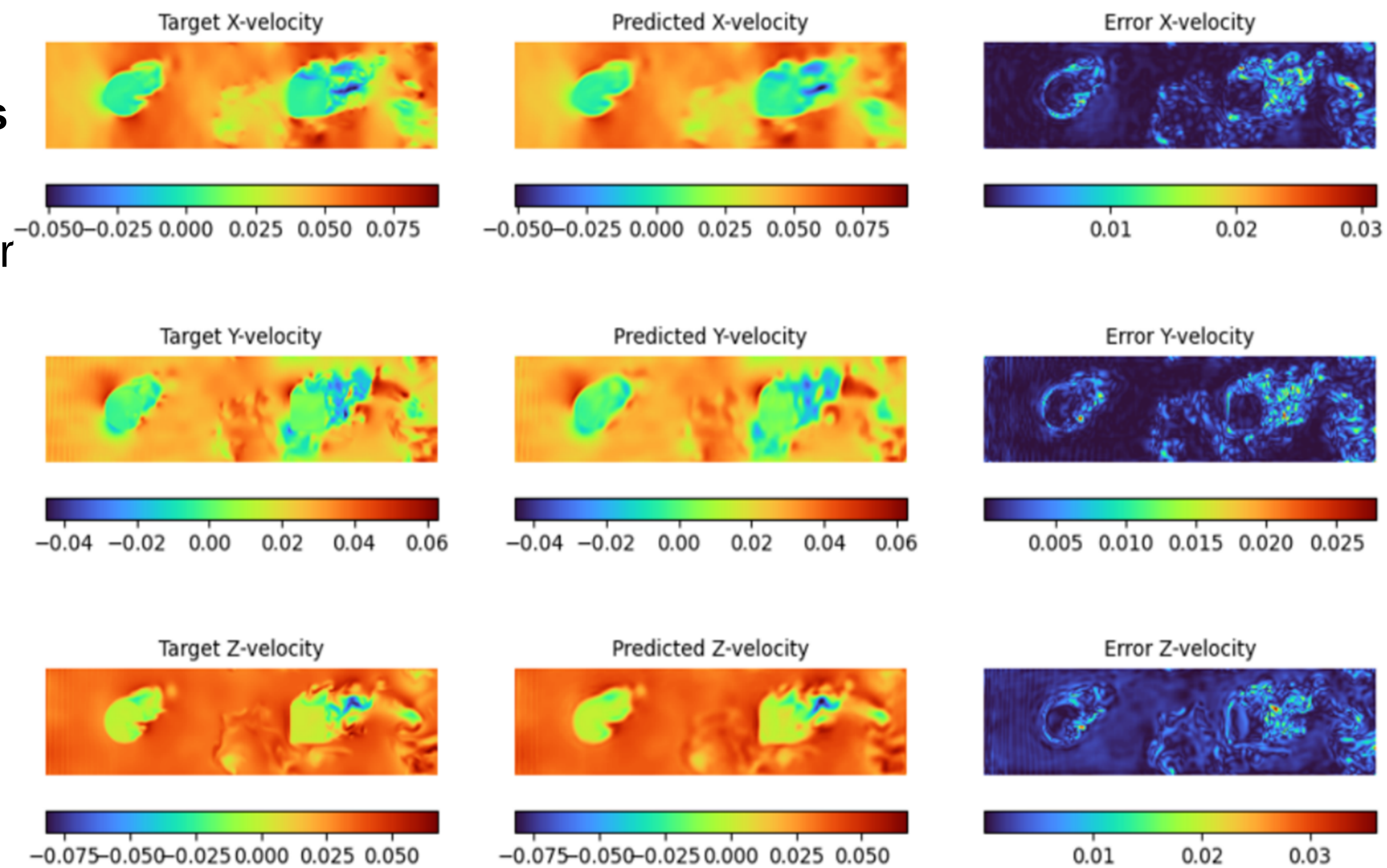
Results and Analysis : Advanced U-Net Model

Model Capacity Evaluation through Overfitting

- Similarly, model is trained for **5000 epochs** using **16 training samples**
- **L1 loss of 0.09** was observed, near to ideal loss of zero.
- **71 % improvement** over standard U-Net
- Model is now **capable enough** to predict the **complex fluid flow** with fair degree of accuracy



Comparison of Target Velocity, Predicted Velocity, and Absolute Error for Each Component for 16 data size

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Results and Analysis

Comparing Relative L1 Norm Error

- ❑ Relative L1 norm error:

$$||E||_1 = \frac{||V_{predicted} - V_{true}||_1}{||V_{true}||_1}$$

$$V_{predicted} = Model\ Prediction$$
$$V_{true} = Ground\ Truth$$

Velocity Component	Relative L1 Norm Error for Std. U-net Model	Relative L1 Norm Error for Advanced U-net Model	Improvement in advanced model over base model
X	0.02789	0.008367	70 %
Y	0.04285	0.010855	75.13 %
Z	0.06850	0.02185	68.10 %

Relative L1 Norm Error for Base and advanced model

Summary

Conclusion

Problem: Minimizing Delay in Design Optimization

- ❑ Useful in industries such as **aerospace and automotive**

Advanced U-Net Based Surrogate Model Development

- ❑ Capable of approximating **complex flow scenarios**
- ❑ Demonstrates the use of **data and model parallelism** for efficiency

Potential to Accelerate the Design Optimization Process

- ❑ Surrogate Model is relatively **less accurate**.

DL Based Surrogate Model + Traditional CFD = Accelerated Design Optimization Process

Early-Stage Design | **Final Validation**

Future Steps

Model Training on Large Dataset

- Training on **10,000 samples** to evaluate the advanced U-Net model's **generalization capabilities**
- An **ablation study** will assess the impact of **architectural** elements

Comparing Surrogate Model with Traditional CFD

- Compare the **accuracy** of the surrogate model against **traditional** methods
- **Analyze convergence time**, highlighting the **total time saved** by using the surrogate model
- Assess **computational resource usage**, including energy consumption

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Thank you for your attention

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Additional Slides

Residual Connections Inside Encoder and Decoder Block

Why it is beneficial to skip connection inside encoder and decoder block

- **Encoder and Decoder Blocks** typically include Convolution, Activation, Batch Normalization, Attention Mechanism, Dropout, and Deconvolution operations.
- Reducing spatial dimensions with strides > 1 in convolution can lead to loss of spatial information, as details from the down sampled regions are not preserved.
- The choice of kernel size and padding influences information capture. Large kernels capture more context but may lose finer details if padding is inadequate
- Activation functions like ReLU or LeakyReLU introduce non-linearity, which is crucial for learning complex patterns. However, they may also lead to information loss by suppressing or zeroing out certain features.
- Batch normalization smooths activations for better training stability but excessive normalization can blur important feature distinctions, potentially leading to a loss of detailed information.
- Attention mechanisms (channel and spatial) highlight important features but may downplay less emphasized ones, potentially resulting in the loss of some information if not carefully managed.

Proposed Future Steps

- **Training on a Larger Dataset**
  - Training datasets will be scaled up to 10,000 samples to evaluate the advanced U-Net model's generalization
  - An ablation study will be conducted to assess the impact of different architectural elements, such as encoder layers, attention mechanisms, and channel size, on the model's performance.

- **Performance Comparison and Hybrid Model Development**
  - We plan to compare the advanced U-Net with the Fourier Neural Operator (FNO) to evaluate differences in accuracy, computational efficiency, and scalability, focusing on capturing fine flow structures, training time, and performance on large-scale problems.
  - Based on this comparison, we aim to develop a hybrid model that combines U-Net's fine-scale feature extraction with FNO's global flow dynamics modeling, improving both accuracy and efficiency in fluid dynamics predictions.

- **Evaluation of Surrogate Models**
  - We will compare the accuracy of the surrogate model (advanced U-Net or hybrid) with traditional CFD methods, focusing on average and maximum errors in critical flow regions.
  - Convergence time will be assessed, with surrogate models expected to significantly outperform CFD simulations, especially in complex, iterative domains.
  - Computational resource usage, including CPU/GPU power, memory consumption, and energy expenditure, will be analyzed to quantify potential cost savings from using surrogate models over traditional CFD.

Skip Connections Inside Encoder and Decoder Block.

Why Use Skip Connections in Encoder-Decoder Blocks?

❑ **Operations with Potential Information Loss**

Convolution

Convoluition with Larg Kernel Size

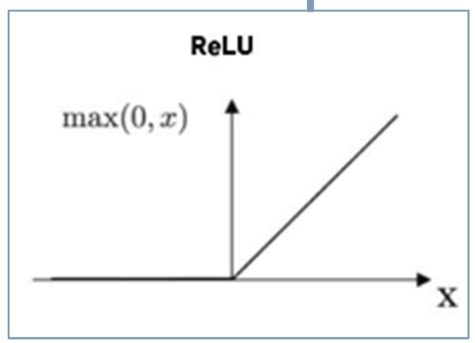
Convolution with Stride > 1

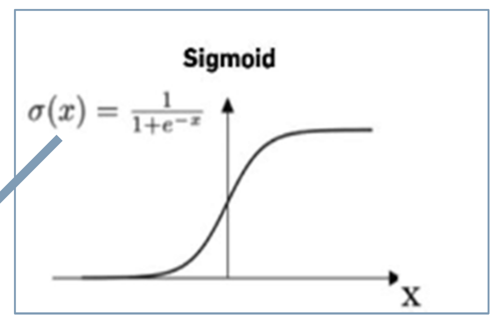
Down Sampling

Reduction of Spatial Resolution

loss of fine-grained details

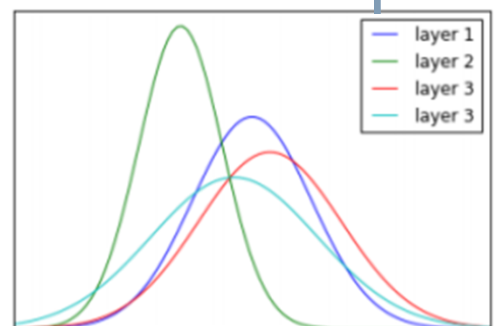
Activation Function





$$\sigma(x) = \frac{1}{1+e^{-x}}$$

Batch Normalization



μ=0 , σ=1

- *blurs the distinctions between features*
- *diminish unique char. of certain features*

Attention Mechanism

Reducing Dimentions:
$C \times H \times W \rightarrow C \times 1 \times 1$
$C \times H \times W \rightarrow 1 \times H \times W$

Loss of Information:
- *Average pooling*
- *Max pooling*

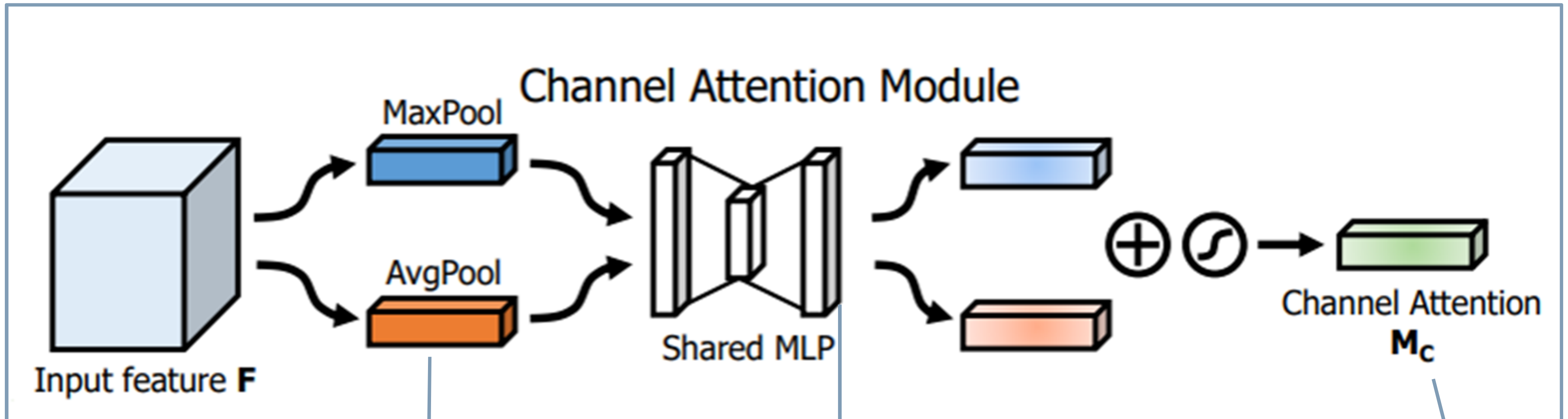
Advanced U- Net Architecture

- ❑ Building upon the standard U-net architecture, we have incorporated additional features in the architecture.

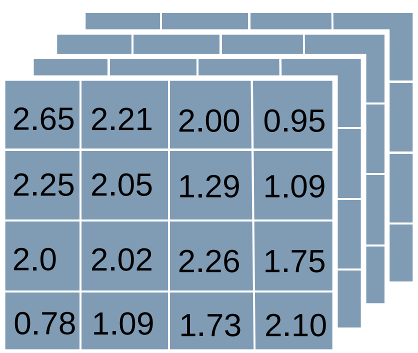
- ❑ **Key Enhancements Over Standard U-Net:**

  - ➢ Encoder layers with varying kernel sizes, maintaining spatial dimensions and channel count
  - ➢ Increased encoder layers and number of channels (up to 4096).
  - ➢ Skip connections within the encoder and decoder block.
  - ➢ Convolution Block Attention Module (CBAM) for improved feature extraction.

Convolution Block Attention Module (CBAM) for improved feature extraction.

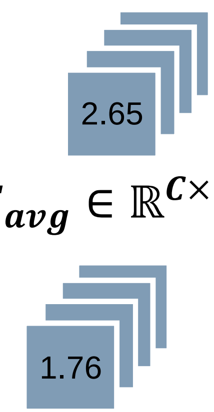


$\boldsymbol{F} \in \mathbb{R}^{C\times H\times W}$



$\boldsymbol{F_{max}} \in \mathbb{R}^{C\times 1\times 1}$

$\boldsymbol{F_{avg}} \in \mathbb{R}^{C\times 1\times 1}$



Capture Inter- Channel Dependancies

$M_c = \sigma(MLP(F_{avg}) + MLP(F_{max}))$

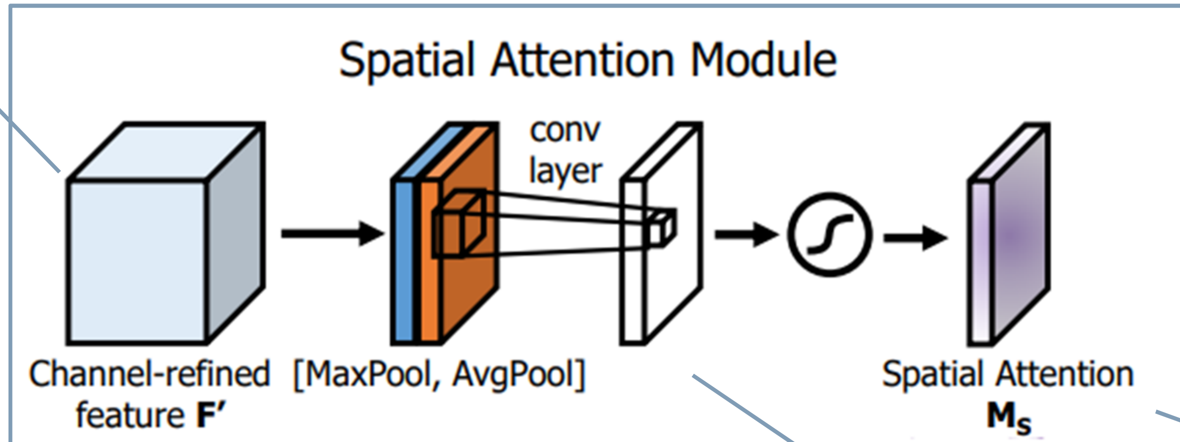
Channel Refined Feature Map: $\boldsymbol{F' = M_c \Theta F}$

Focus : What ?

Convolution Block Attention Module (CBAM) for improved feature extraction.

$\boldsymbol{F'} \in \mathbb{R}^{\boldsymbol{C \times H \times W}}$

2.65	2.21	2.00	0.95
2.25	2.05	1.29	1.09
2.0	2.02	2.26	1.75
0.78	1.09	1.73	2.10



$\boldsymbol{F'_{max}} \in \mathbb{R}^{\boldsymbol{1 \times H \times W}}$

2.15	2.21	2.00	0.95
2.25	2.5	1.29	1.59
2.05	2.32	2.26	1.75
1.78	1.89	2.73	2.86

$\boldsymbol{F'_{avg}} \in \mathbb{R}^{\boldsymbol{1 \times H \times W}}$

1.56	2.21	2.00	0.95
2.25	2.65	1.79	1.79
2.0	1.02	2.26	1.65
1.38	1.39	1.73	1.75

$(F'_{max} \,;\, F'_{avg})$

Concatenation $[\mathbb{R}^{\boldsymbol{H \times W \times 2}}]$

$M_s = \sigma(Conv([F'_{avg} \,;\, F'_{max}]))$

Spatial Refined Feature Map: $F'' = M_s \Theta \boldsymbol{F'}$

Focus : Where ?

$$\mathbf{Final\ Output(F'') = Spatial\_Attention(Channel\_Attention(F))}$$

Challenges and Proposed Future Steps

❑ Training on a Larger Dataset

- Training datasets will be scaled up to 10,000 samples to evaluate the advanced U-Net model's generalization
- An ablation study will assess the impact of various architectural elements

❑ Hybrid Model Development

- Compare the advanced U-Net with the Fourier Neural Operator (FNO) to assess differences in accuracy, computational efficiency, and scalability.
- Aim to develop a hybrid model that combines U-Net's feature extraction with FNO's global flow dynamics modeling to improve accuracy and efficiency.

❑ Comparing Surrogate Model with Traditional CFD

- compare the accuracy of the surrogate model (advanced U-Net or hybrid) with traditional CFD methods
- Analyze computational resource usage, including CPU/GPU power and memory consumption, to quantify cost savings from using surrogate models over traditional CFD