

um
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Geometric Deep Learning for Surrogate Modeling

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Agenda

Surrogate modeling for geometrically varying domains

Challenges in real-world scenarios

Modular non-parametric surrogate framework

Implicit geometry representation

Use case - DrivAer

Numerical setup and parametrization

End-to-End Deep Learning Approach

Integral values and fields predictions

Conclusions



Surrogate modeling for geometrically varying domains



Problem Setting

Surrogate models are widely used to accelerate many-query or real time processes like design exploration, optimization and uncertainty quantification.

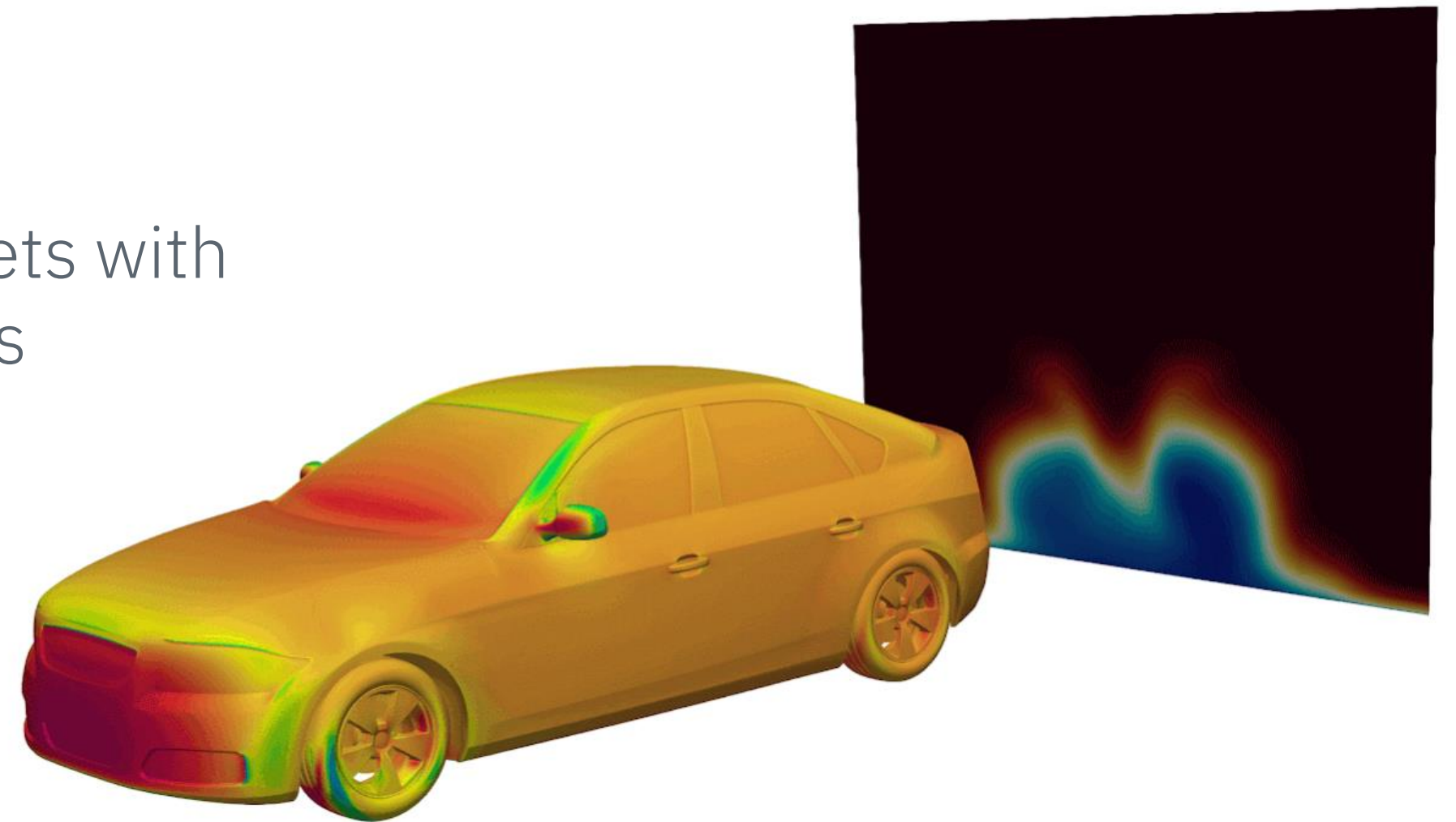
However, some real-world scenarios may introduce additional challenges in presence of **geometrically varying domains**.

- **Geometric parameterization:**

Geometries may originate from legacy datasets with inconsistent or unavailable parameterizations

- **Mesh representation:**

Meshes may lack point-to-point correspondence, or even differ in topology

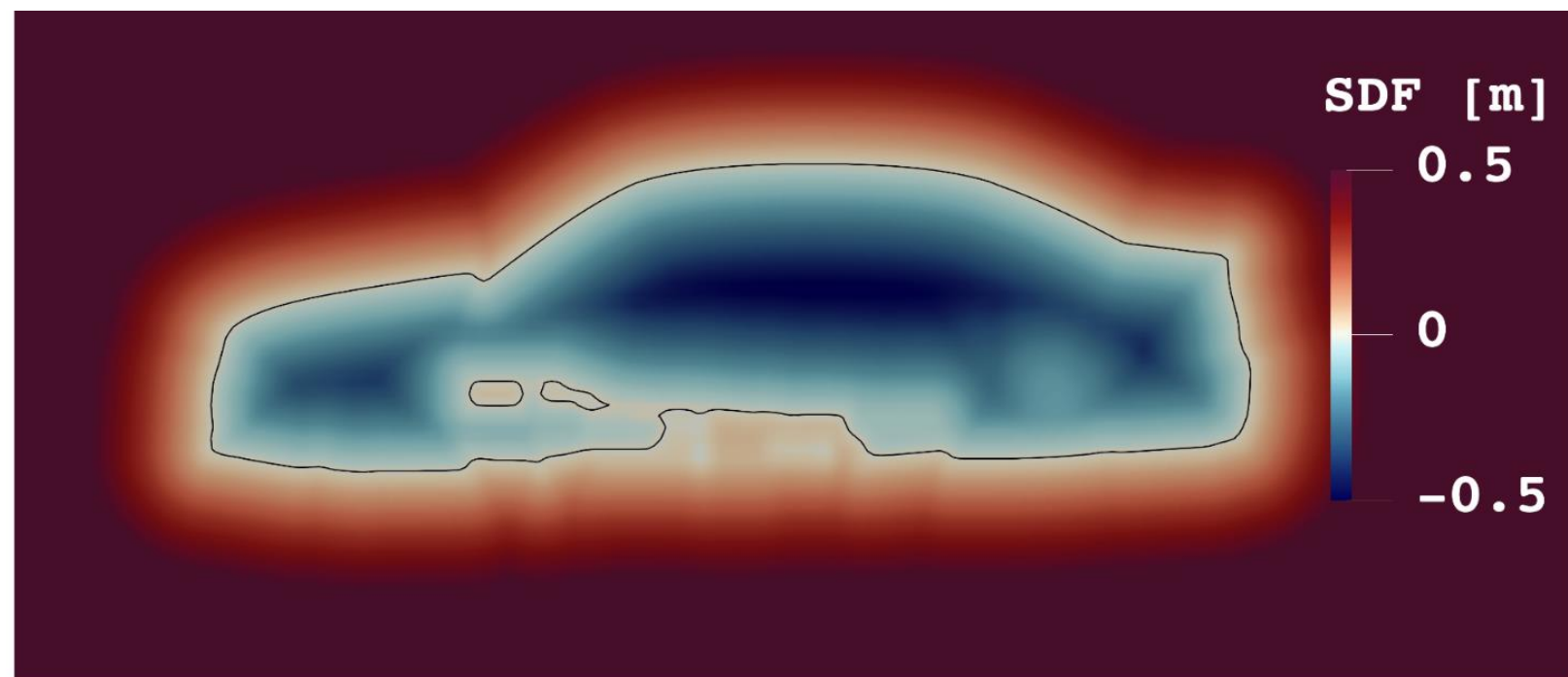


A modular non-parametric surrogate framework

Goal: geometric deep learning techniques to develop a **mesh- and parametrization-free framework**

Our approach:

- implicitly represents geometries through their **Signed Distance Functions (SDFs)**

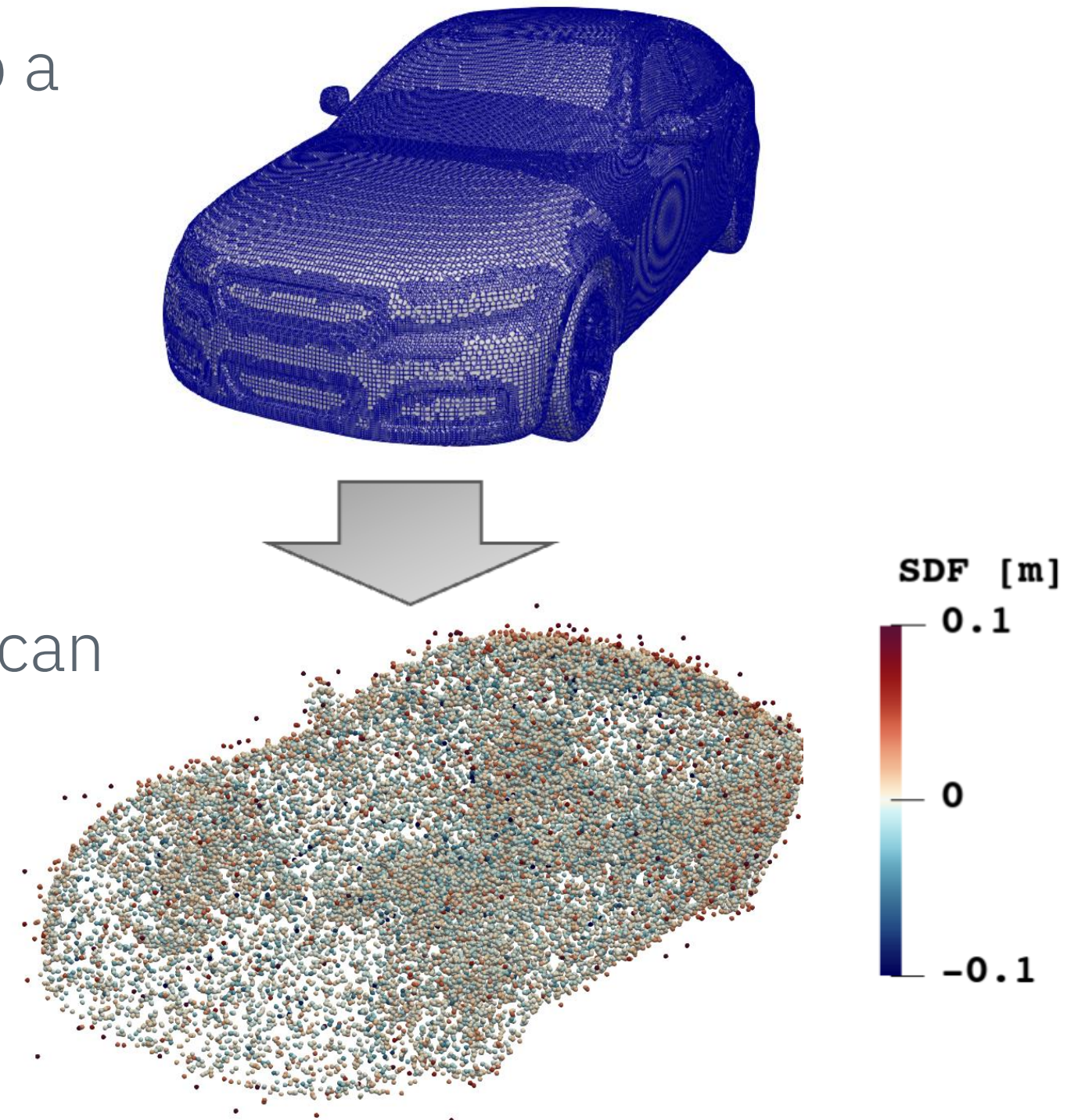


A modular non-parametric surrogate framework

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- enables a **mesh-independent** representation that can be generated **directly from CAD** models

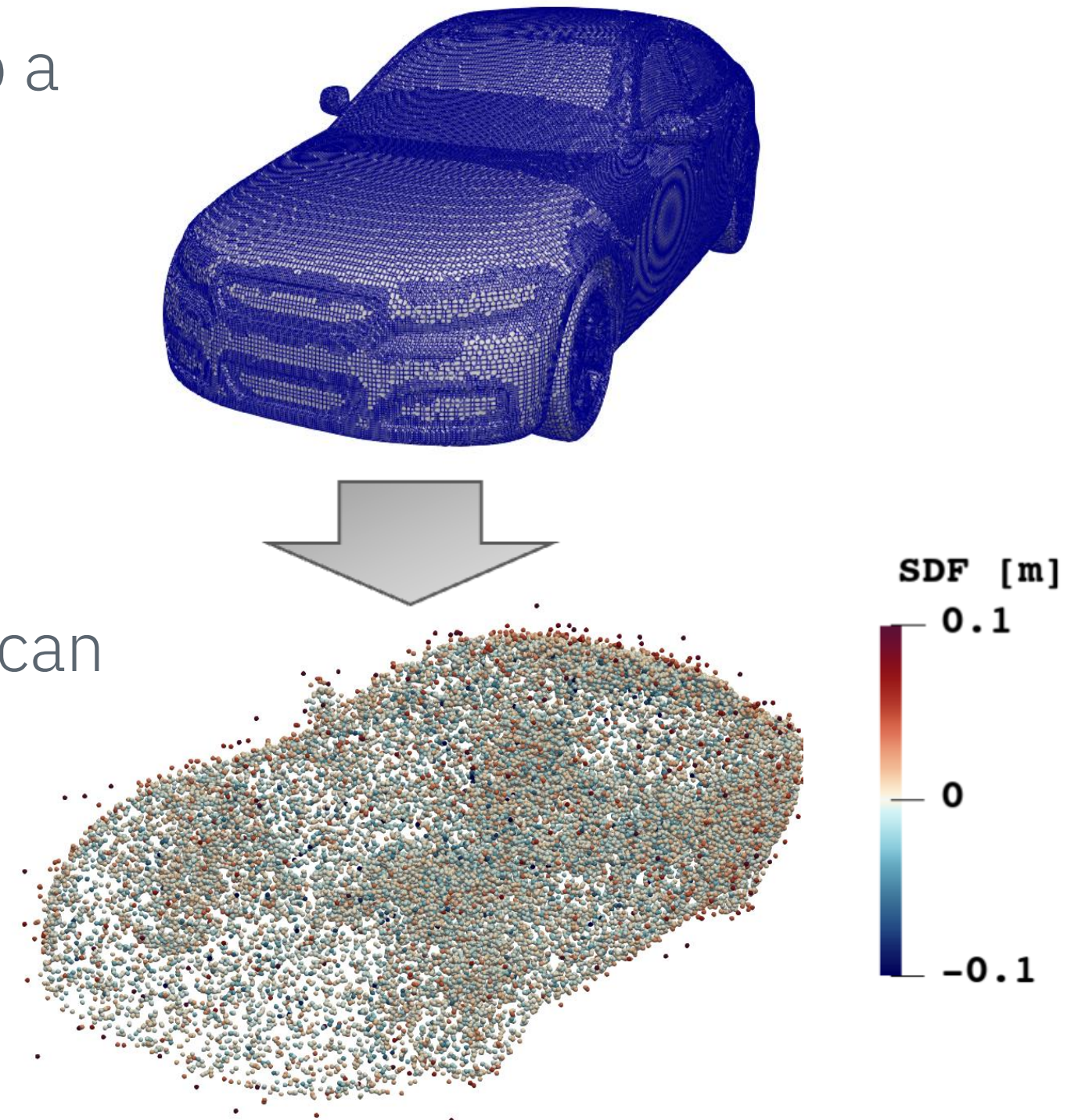


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- **learns a compact latent parametrization** directly from the SDFs

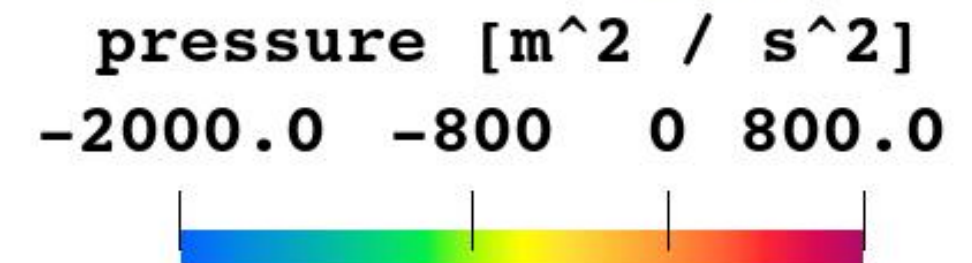
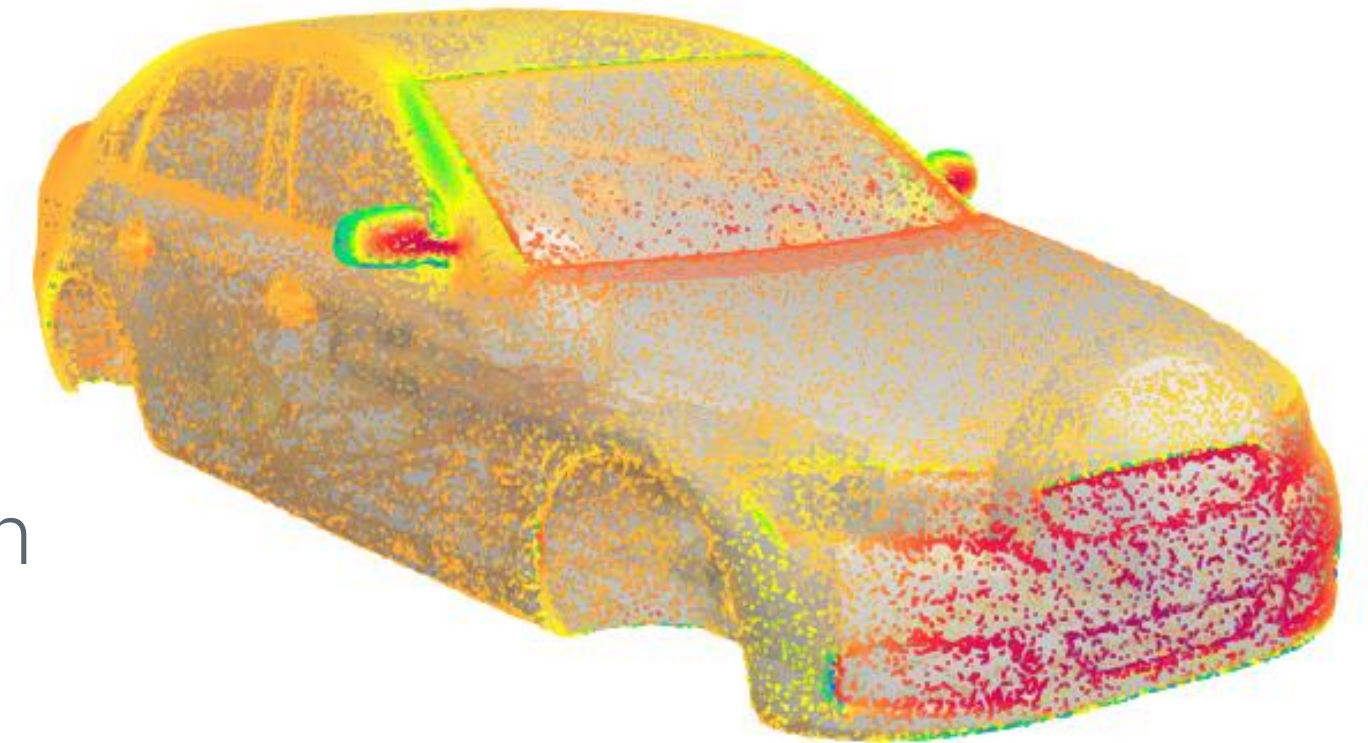


A modular non-parametric surrogate framework

Goal: geometric deep learning techniques to develop a **mesh- and parametrization-free framework**

Our approach:

- implicitly represents geometries through their **Signed Distance Functions (SDFs)**
- enables a **mesh-independent** representation that can be generated **directly from CAD** models
- **learns a compact latent parametrization** directly from the SDFs
- **predicts solution fields** at arbitrary space/time locations from the latent representations



Implicit geometry representation

Main idea: a deep neural network learns a compact shape encoding from the Signed Distance Function representation of the geometry.

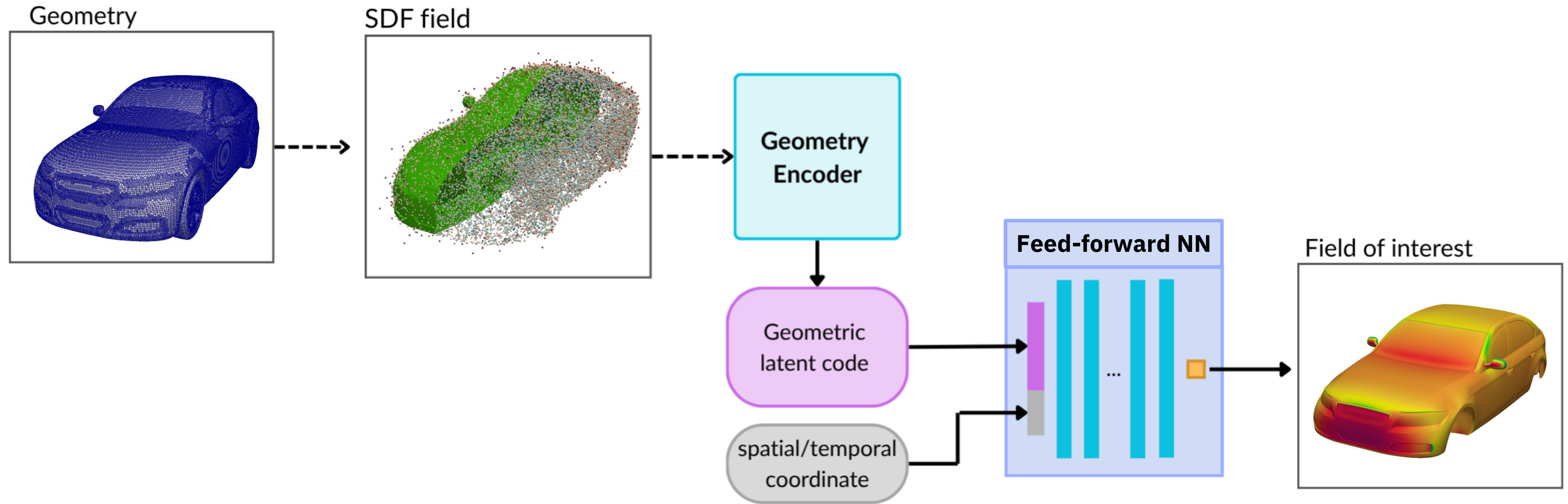
Training

- **Trained on a collection of shapes** represented as Signed Distance Functions (SDFs)
- Learns a fixed-size vector (***latent code***) that **encodes the shape of each geometry**.

Inference

- Finds the latent code **representing a new geometry**
- Solved as an **optimization problem** (almost real-time)

Complete workflow

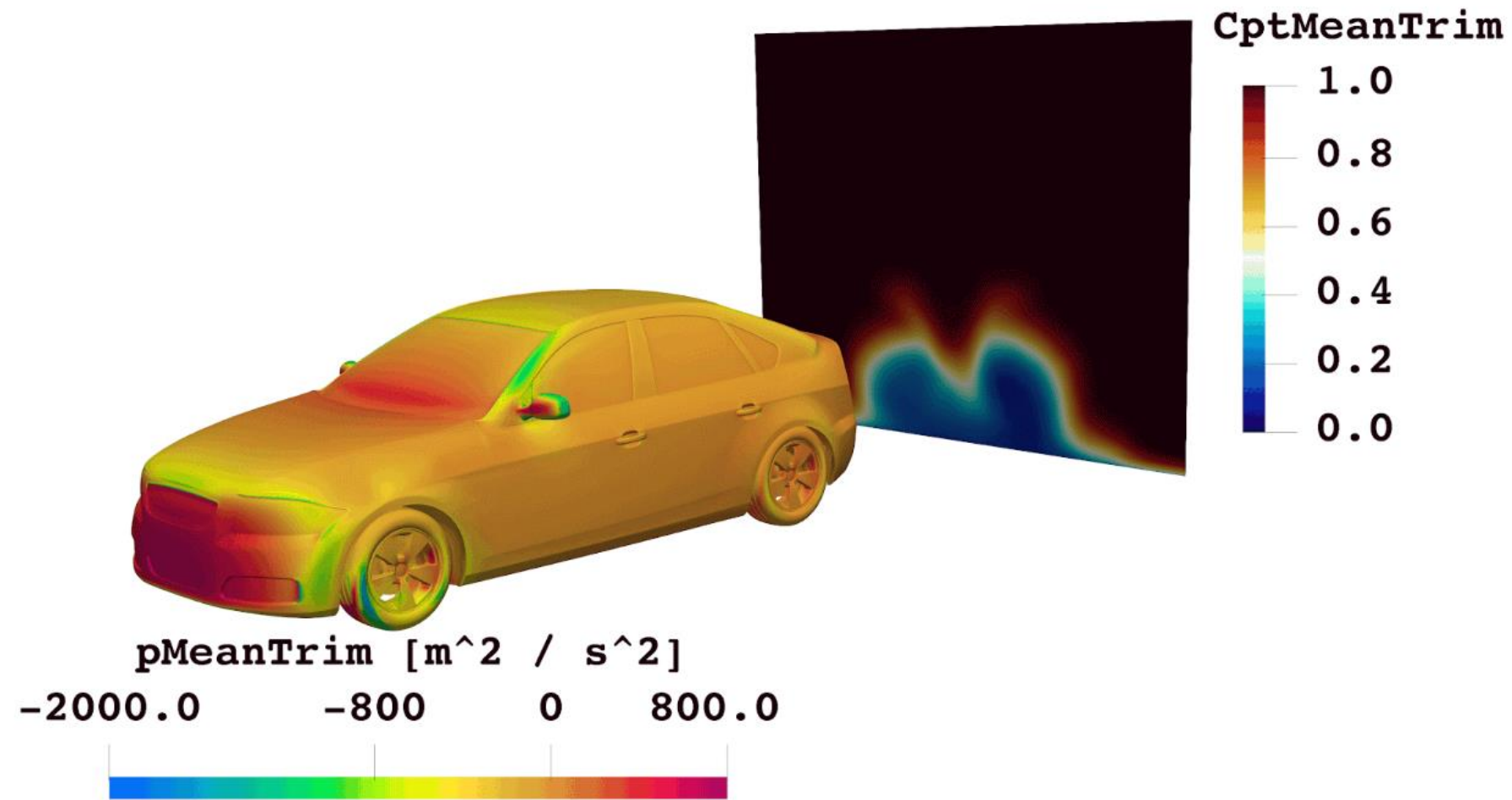


USE CASE - DrivAer



DrivAer Notchback

Numerical Setup & Parameterization



Public Dataset available on Hugging Face:
[neashton/drivaerml](https://huggingface.co/datasets/neashton/drivaerml) · [Datasets at Hugging Face](https://huggingface.co/datasets)

Numerical Setup

Flow Regime

Turbulent Incompressible Flow (DDES with WF)

Mesh Size

~160 million cells

Convergence

±1.5 drag counts

Geometry & DOE

Morphing Param.

16

DOE Samples

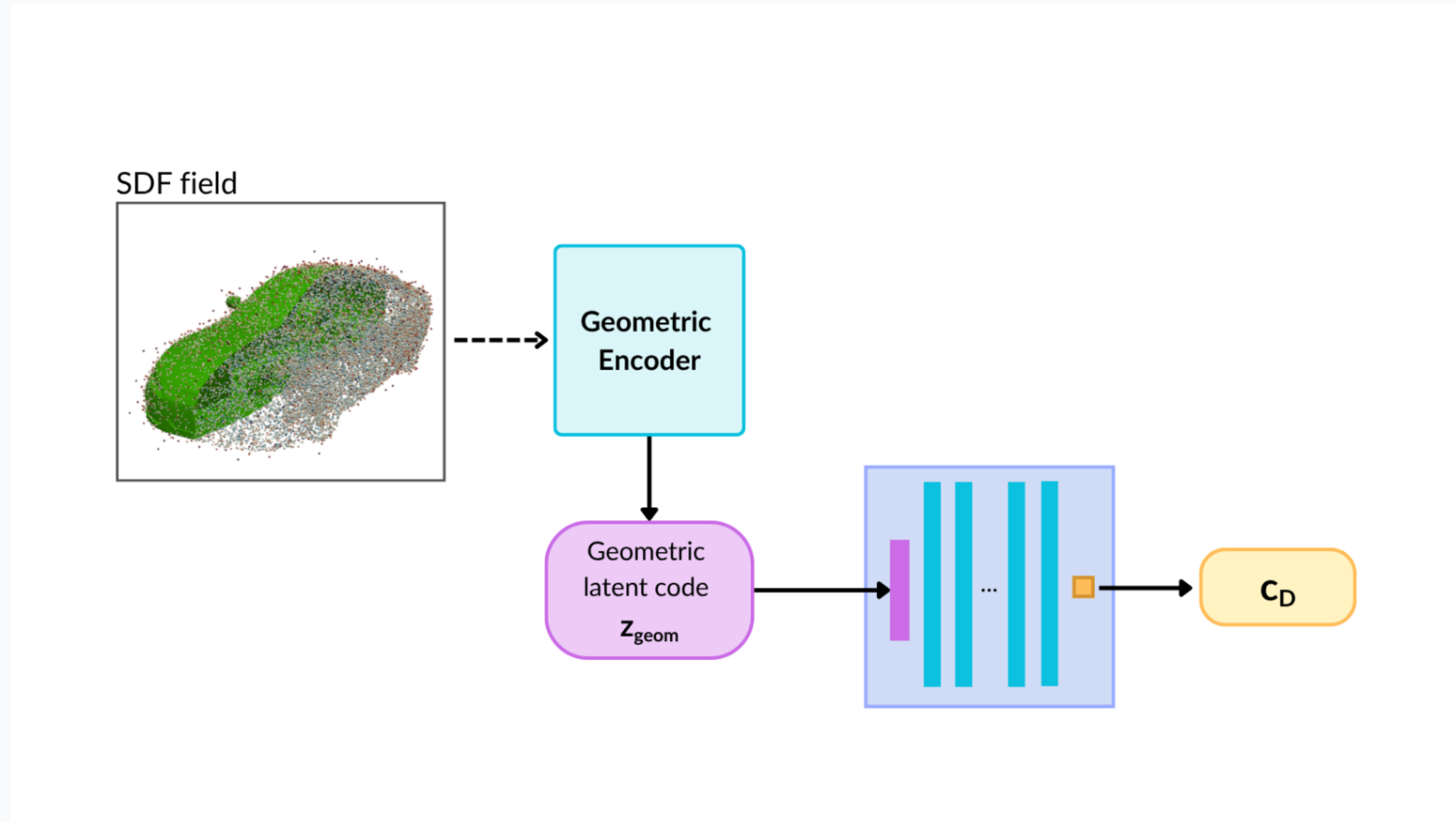
500 (MELS algorithm)

Runtime

~40 h (1,536 CPU cores)

End-to-End Deep Learning Approach

Modular Workflow

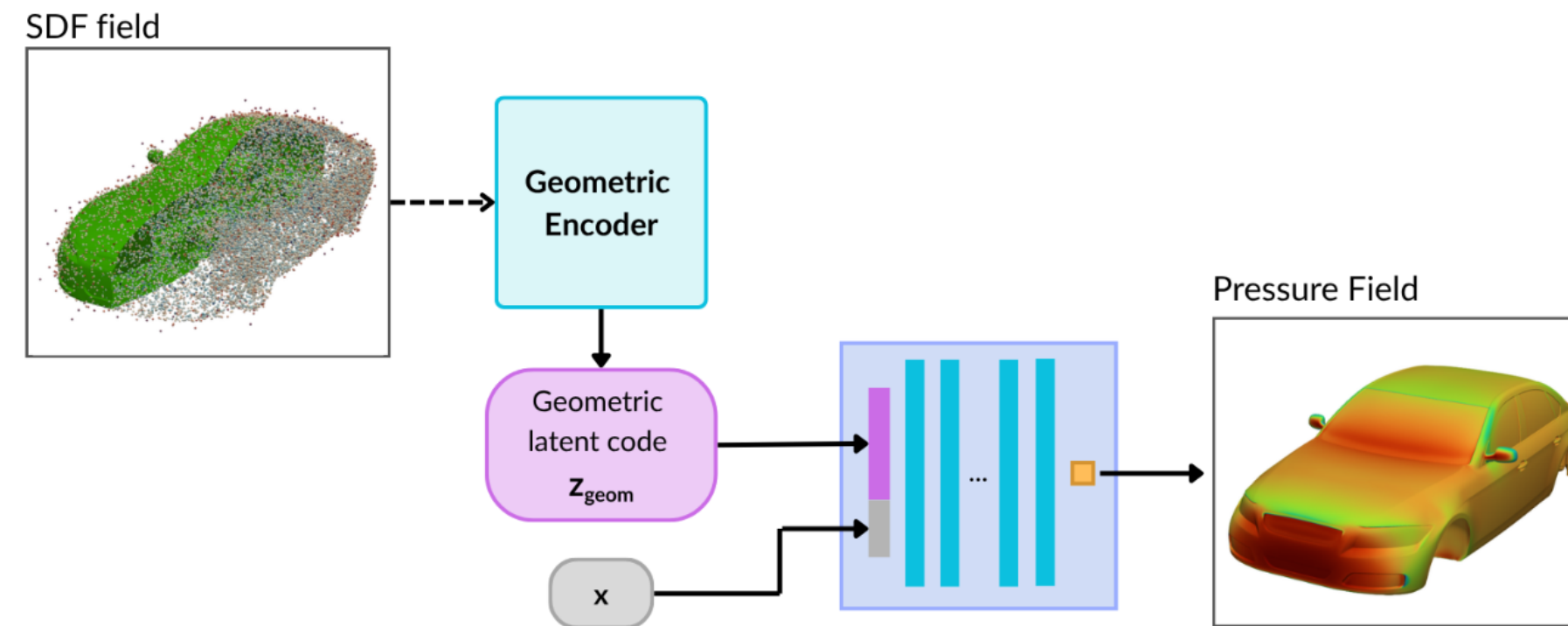


Workflow Overview

1. Integral Workflow

End-to-End Deep Learning Approach

Modular Workflow

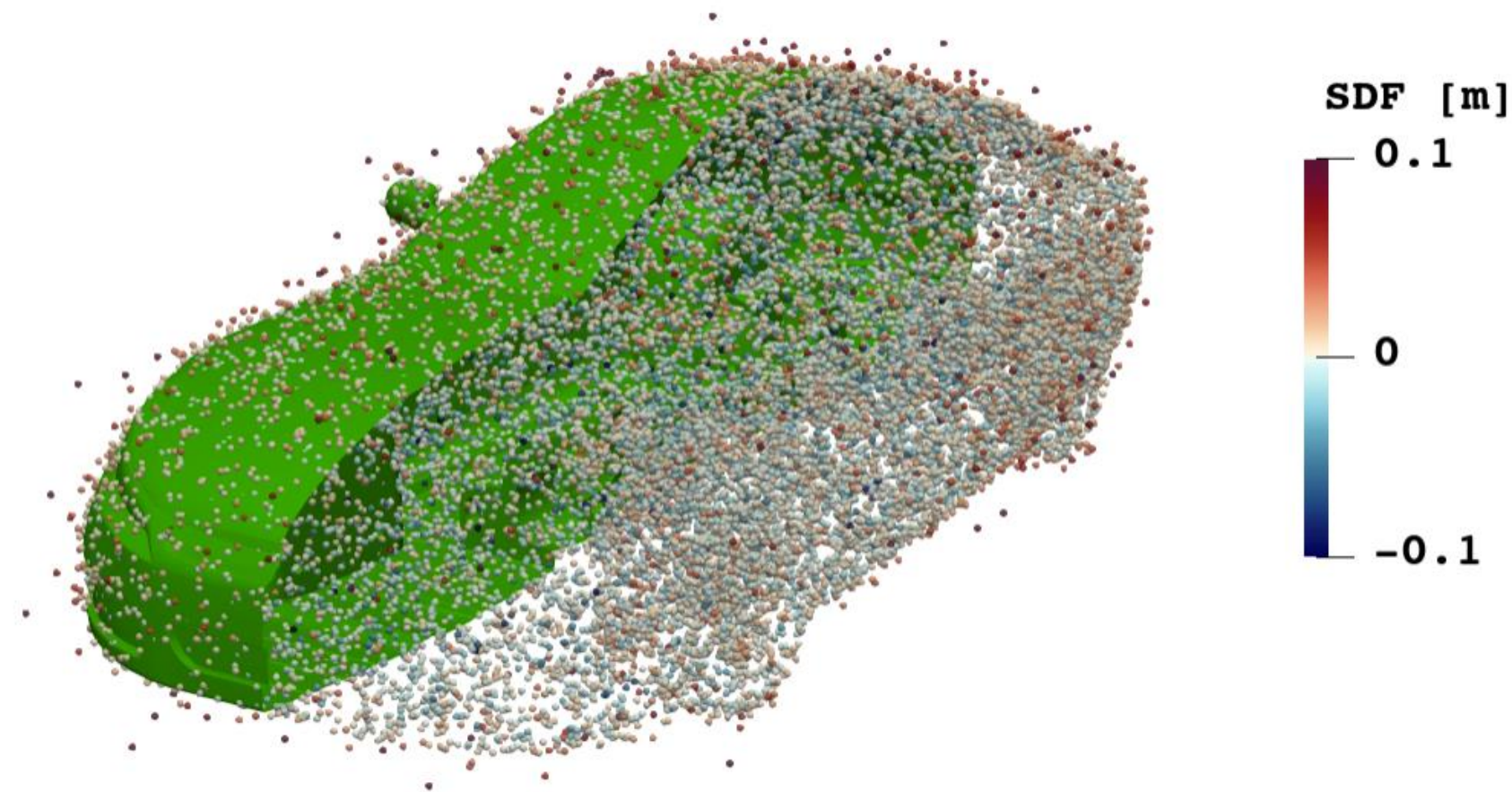


Workflow Overview

1. Integral Workflow
2. Field Workflow

Signed Distance Function

Geometry representation

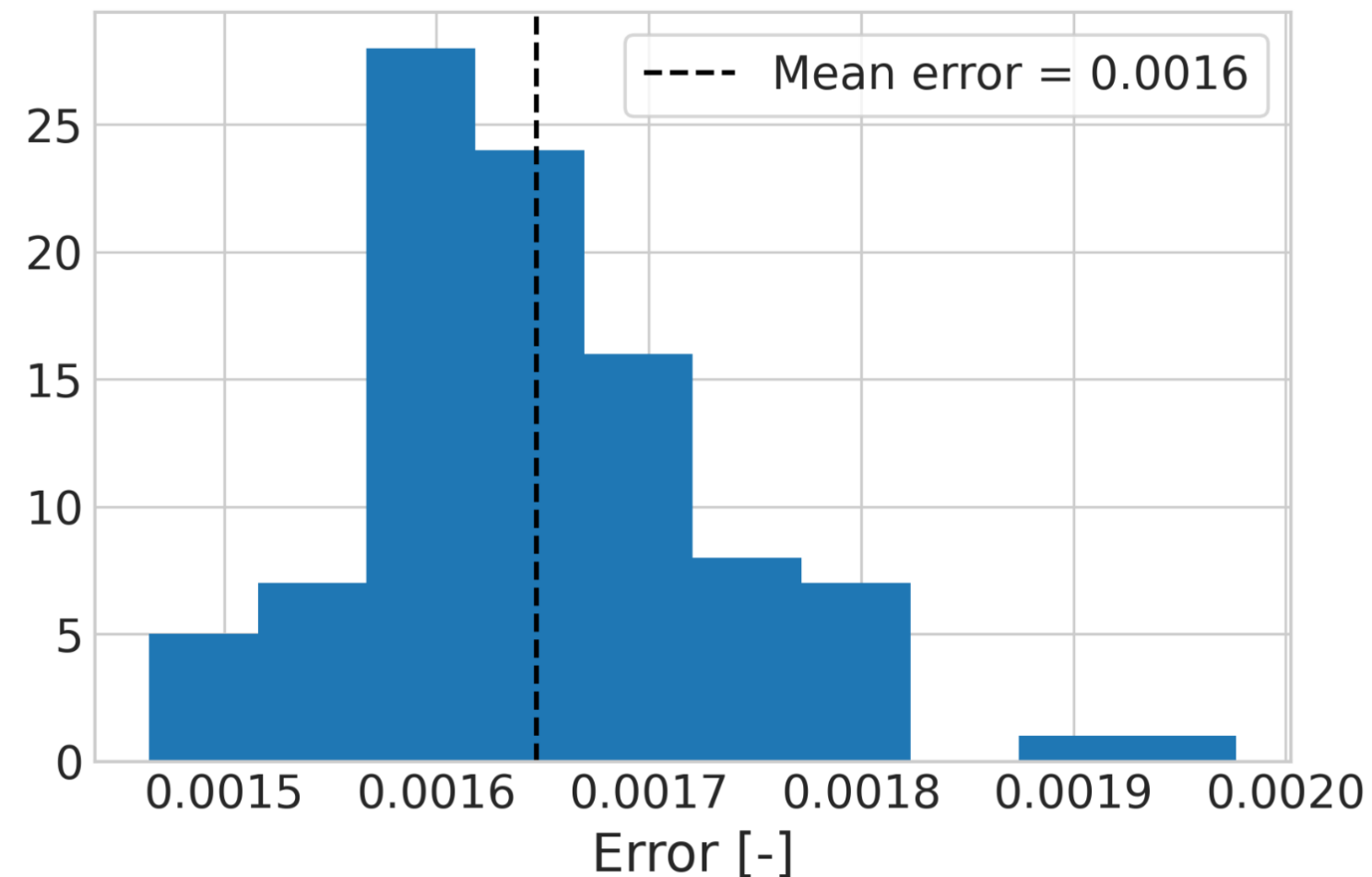


Given a point cloud, the **SDF** provides an **implicit representation** of the geometry by assigning to each point its distance from the object surface.

- **35K points** for each geometry
- dense sampling near the surface

Geometric Encoder

Test Error and Computational Performance



Distribution of mean reconstruction error on unseen samples

Training Setup

Hardware
NVIDIA A10 GPU
24 GB GDDR6, Ampere

Train / Test split
80 / 20
Samples percentage

Data Scale
~14.4M points
Processed per epoch

Model Size
1.06M
Network parameters

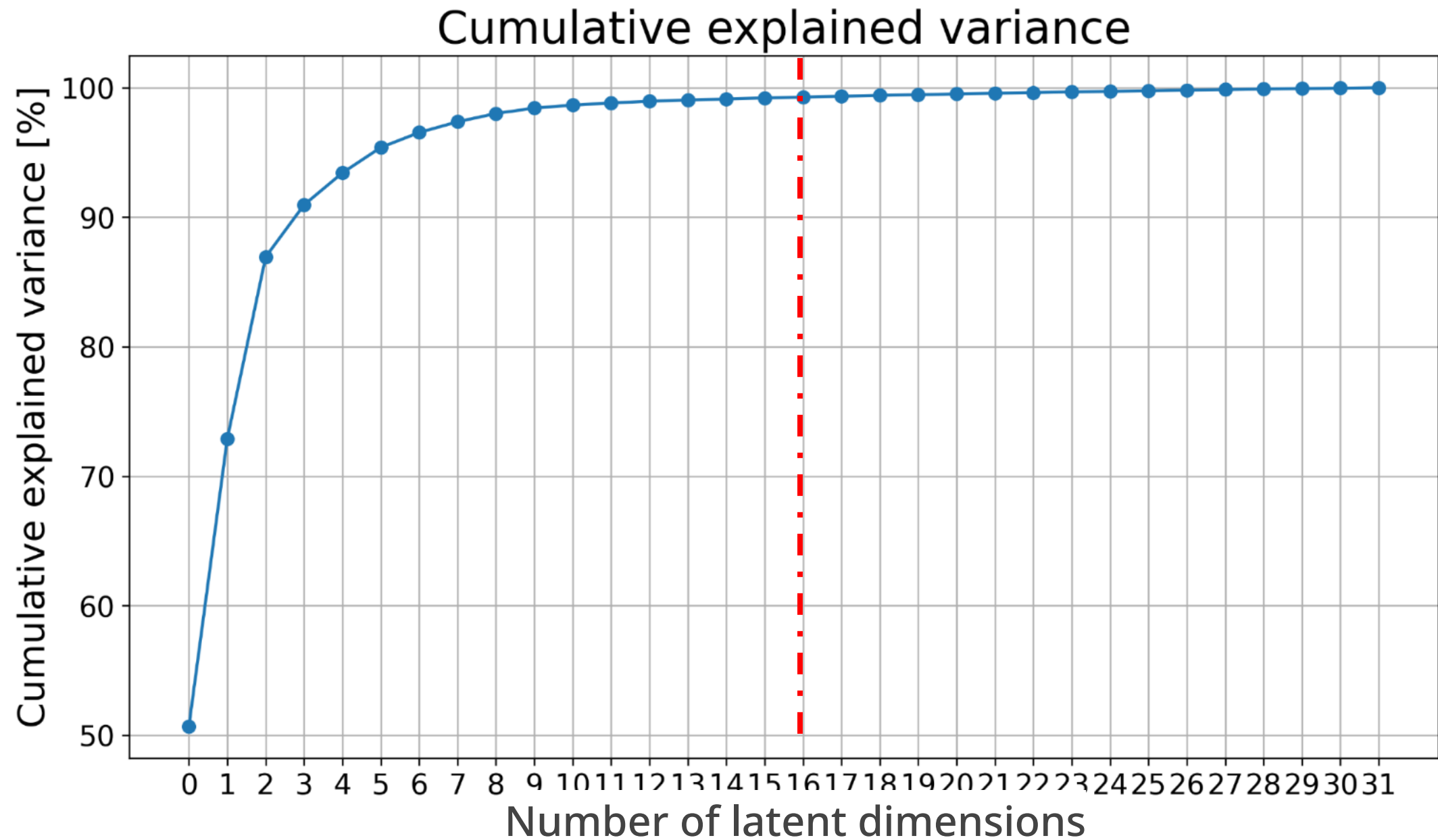
Performance

~10.28 s
per epoch

~5h 42m
total training time
(2000 epochs)

Geometric Encoder

Dimensionality of the Learned Representation



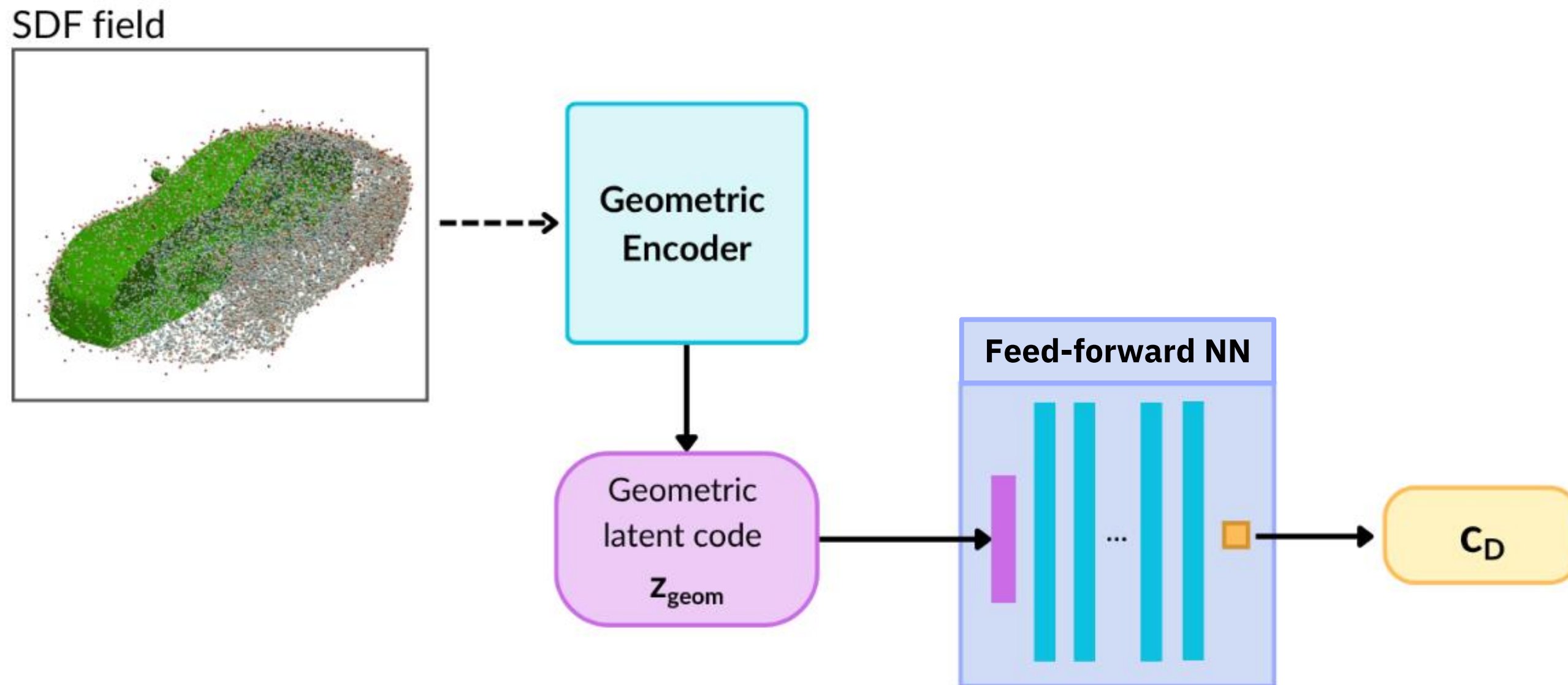
Key Insight

Our model reveals that **~16 latent dimensions** are needed to explain almost all the variance.

This is achieved despite the model learning a more complex **32-dimensional representation**.

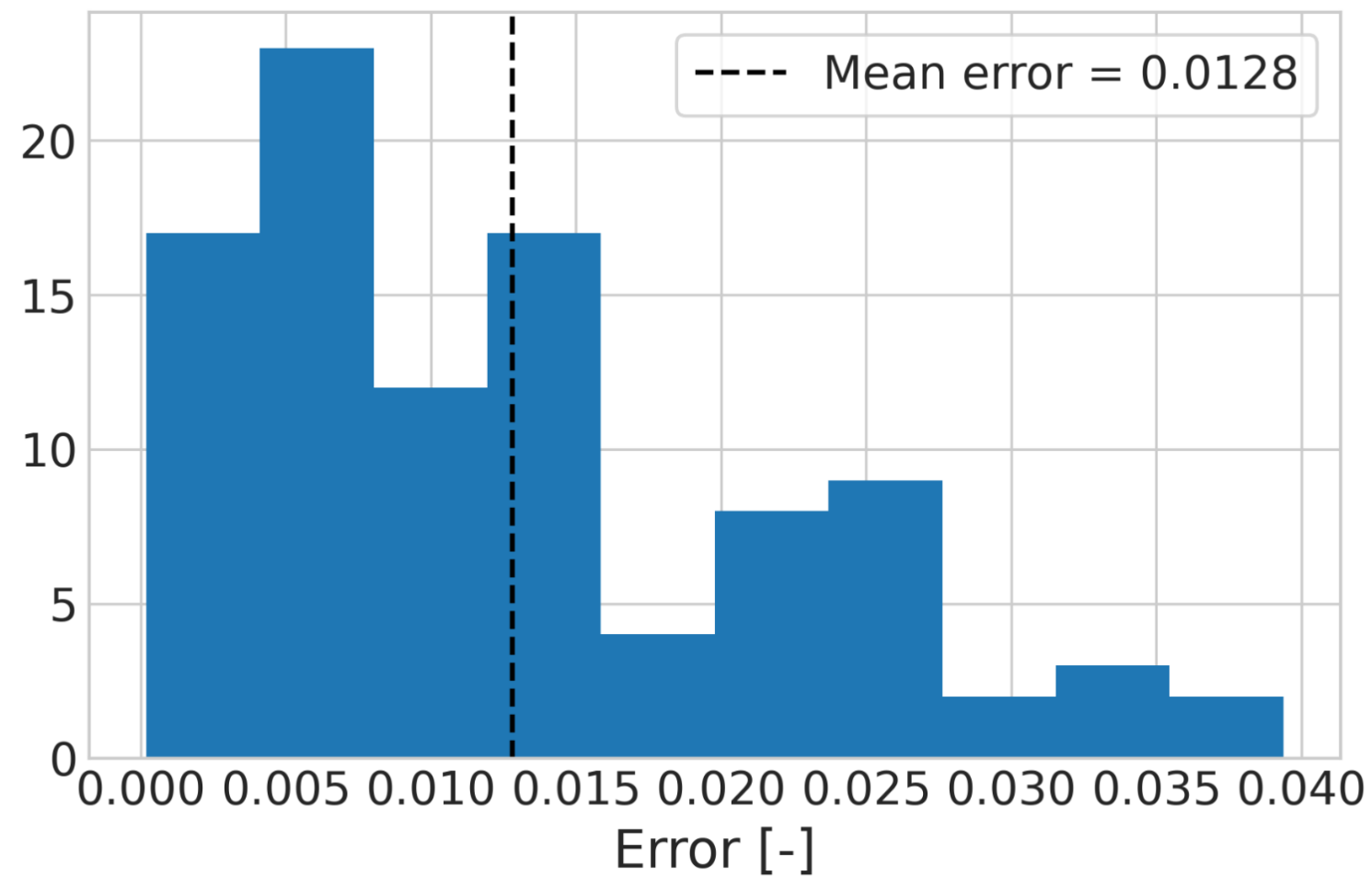
Drag Coefficient Prediction

Integral prediction Workflow



Drag Coefficient Prediction

Test Error and Computational Performance



Distribution of relative error on unseen samples

Training Setup

Hardware
CPU

Train / Test split
80 / 20
Samples percentage

Data Scale
310 cases
Processed per epoch

Model Size
593
Network parameters

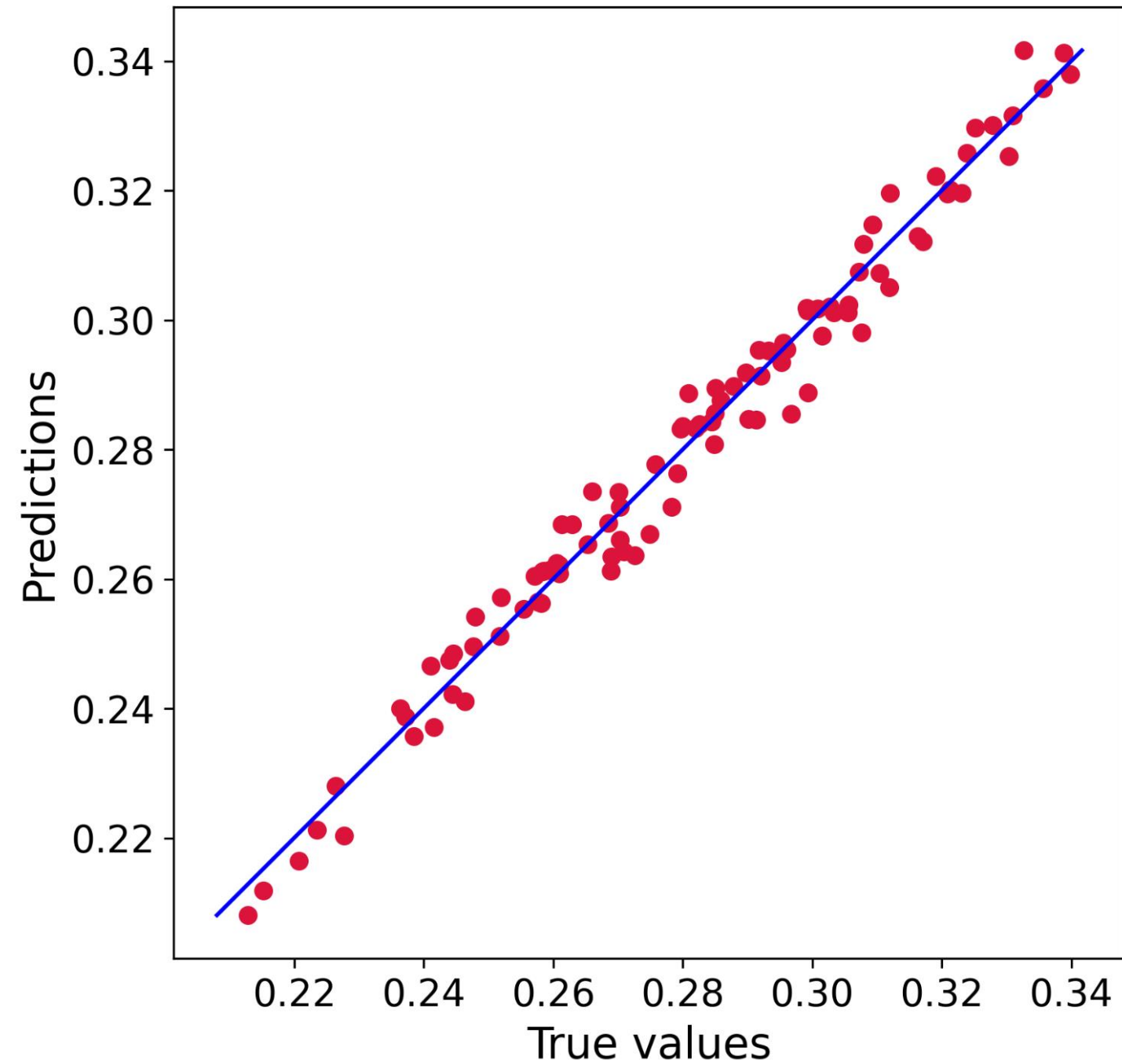
Performance

~0.1 s
per epoch

~3min 32s
total training time
(2000 epochs)

Drag Coefficient Prediction

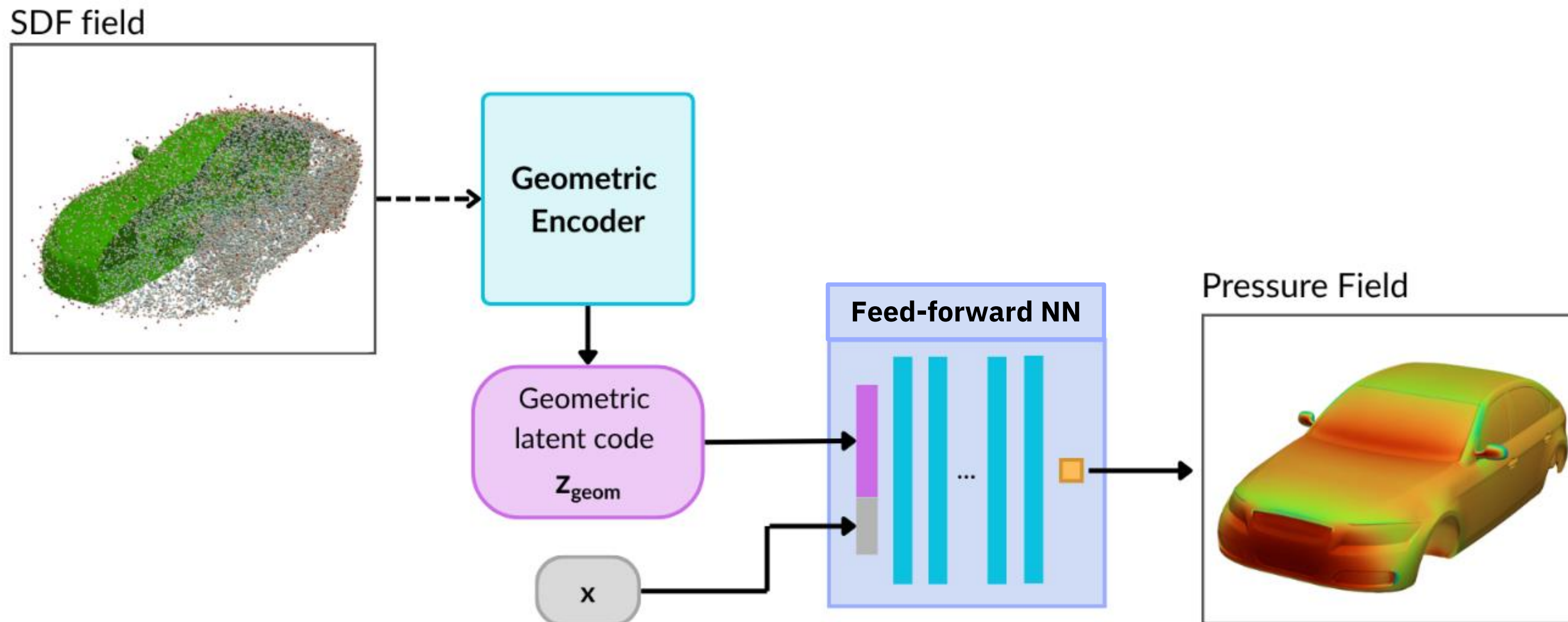
Prediction vs Ground Truth



Comparison of **Ground Truth** vs **Prediction** for the drag coefficient calculated over the test dataset.

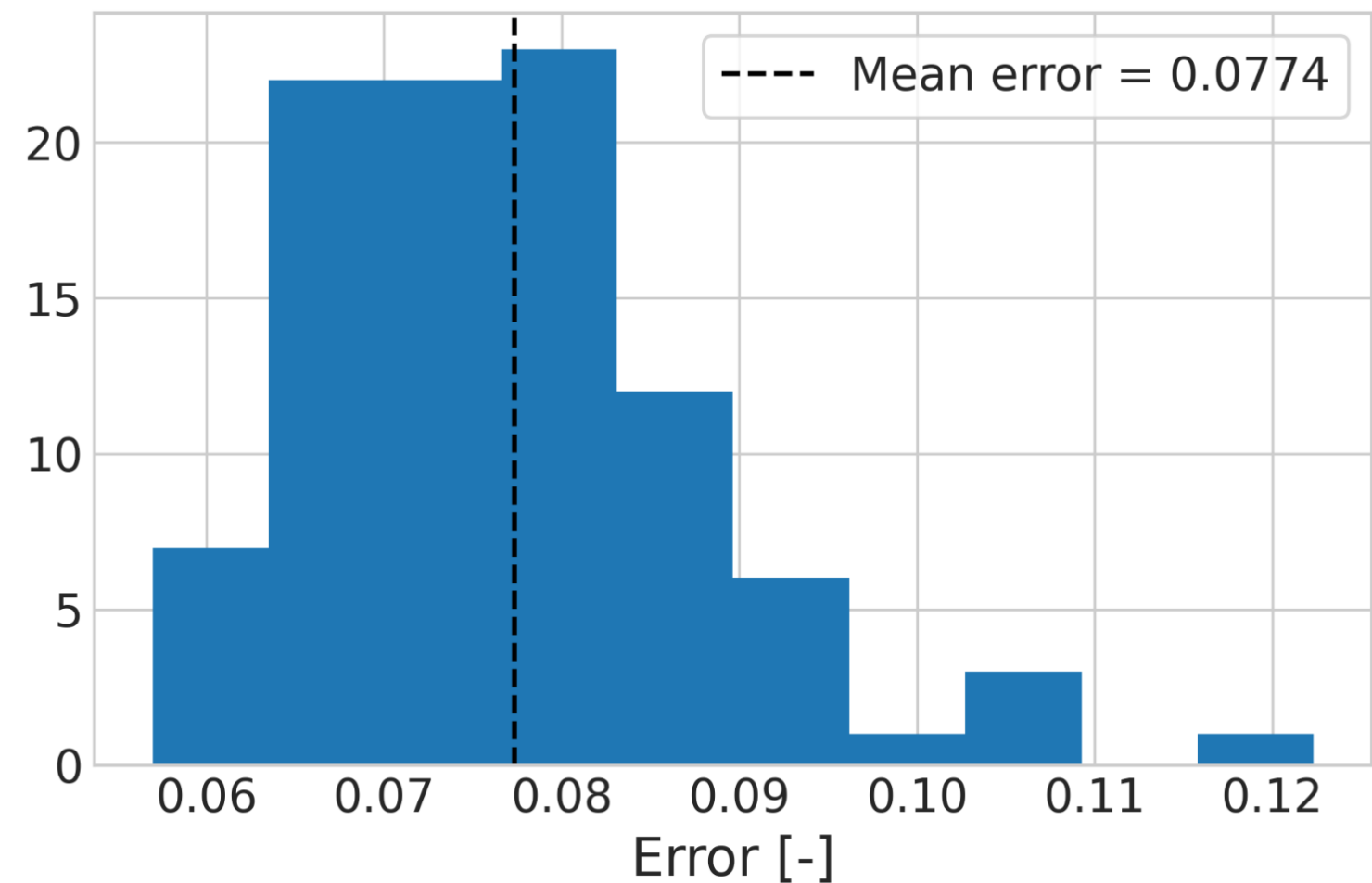
Pressure Field Prediction

Field prediction Workflow



Pressure Field Prediction

Test Error and Computational Performance



Distribution of mean relative error on unseen samples

Training Setup

Hardware
NVIDIA A10 GPU
24 GB GDDR6, Ampere

Train / Test split
80 / 20
Samples percentage

Data Scale
~15.5M points
Processed per epoch

Model Size
1.34M
Network parameters

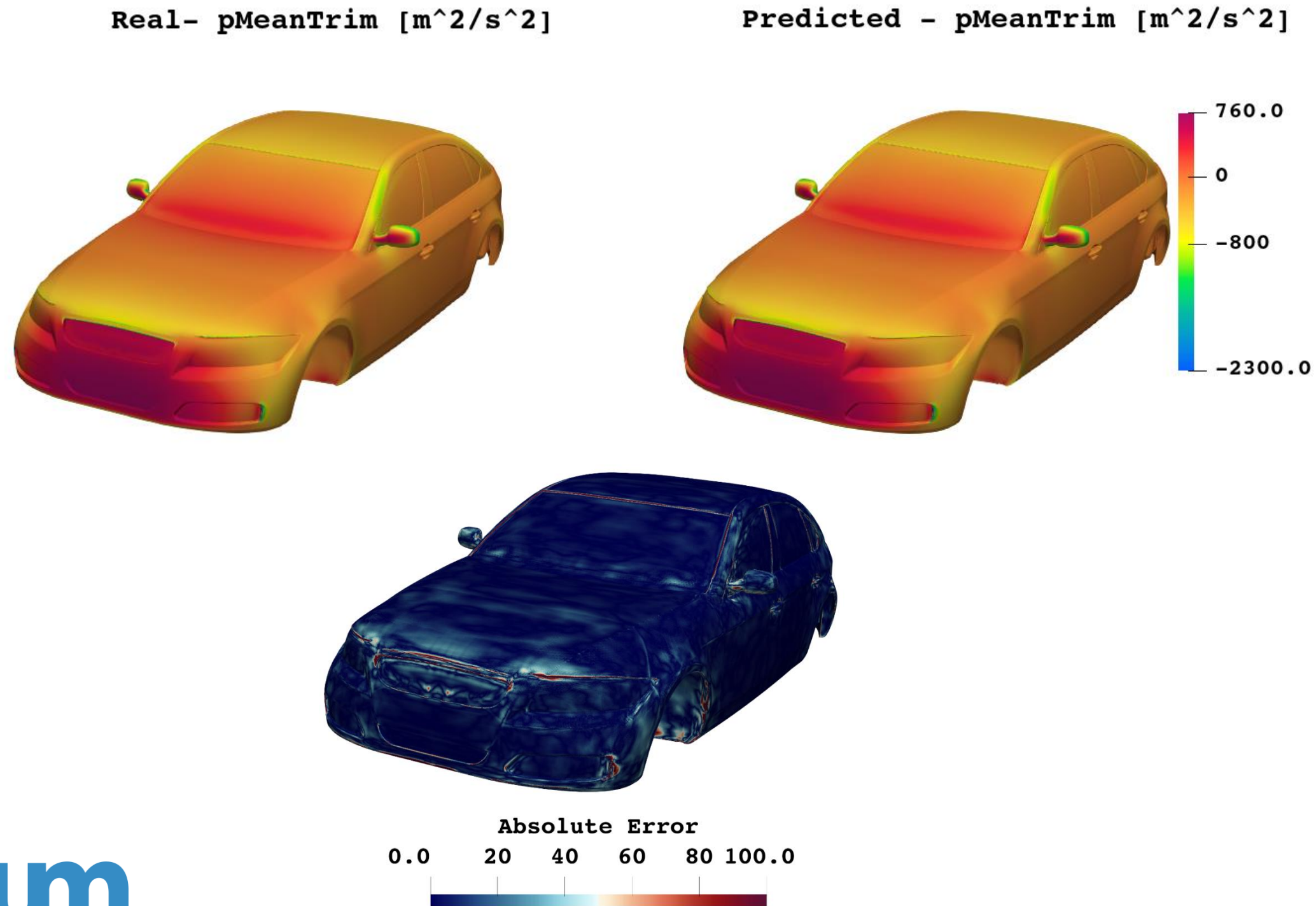
Performance

~16.11 s
per epoch

~8h 57m
total training time
(2000 epochs)

Pressure Field Prediction

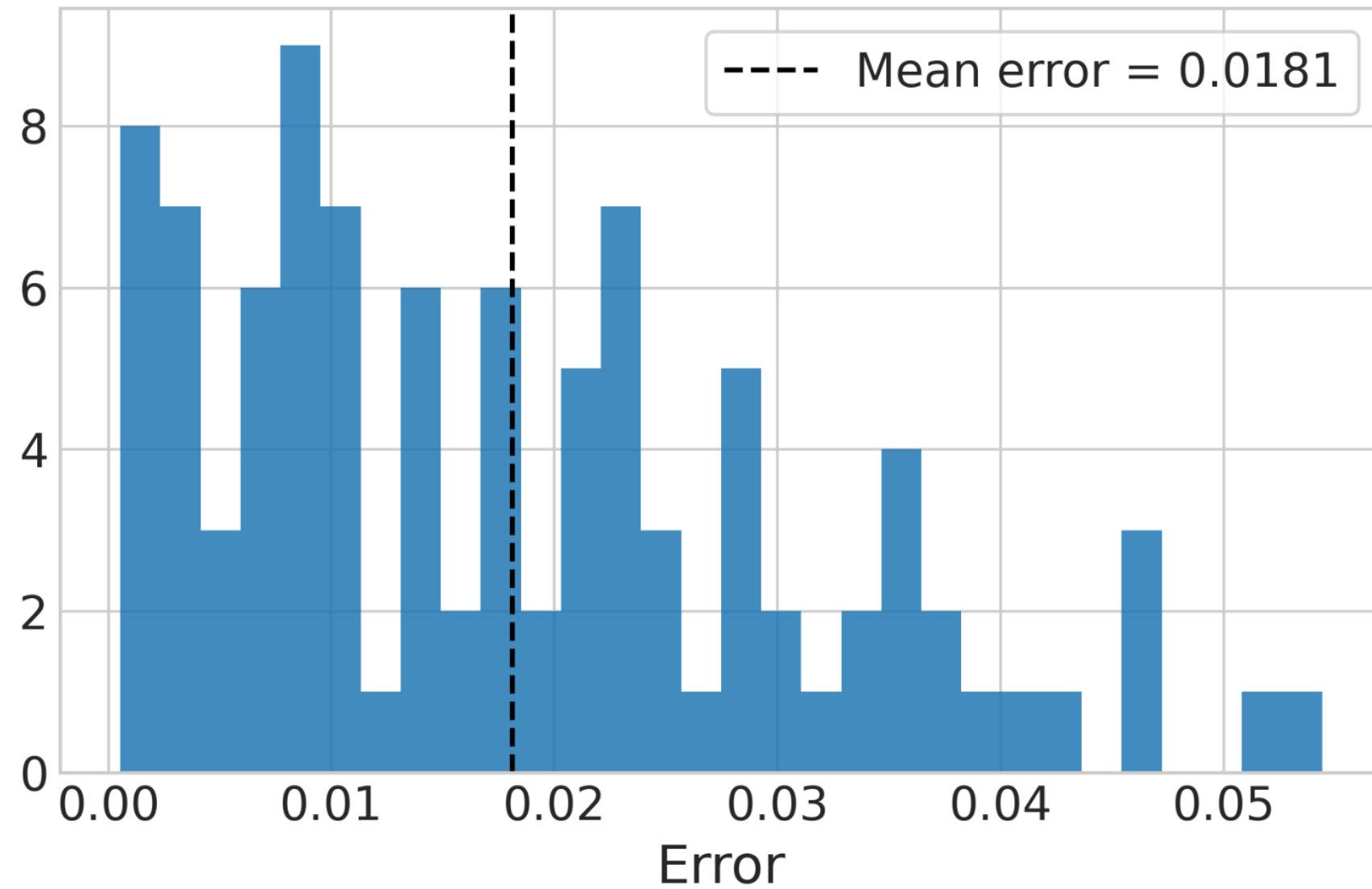
Prediction vs Ground Truth — Median Error Case



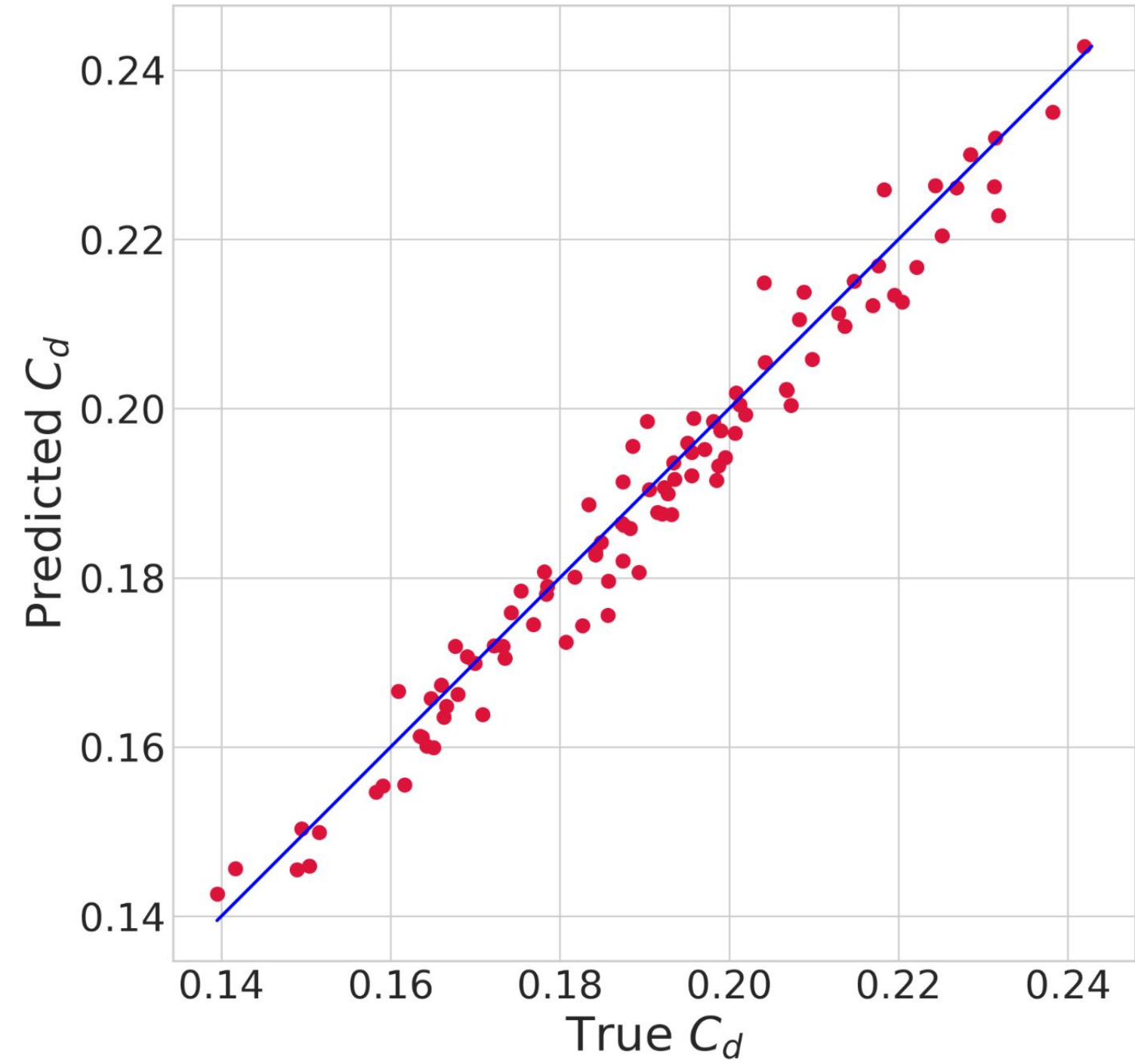
Surface pressure field comparison (**ground truth** vs **prediction**), shown for a case representative of the **median test error** ($\approx 7.56\%$).

Pressure Field Prediction → Drag Coefficient

Drag Coefficient Evaluation and Relative Errors



Distribution of relative error on unseen samples



CONCLUSION

- We presented a **surrogate framework for geometrically varying domains** without mesh correspondence or explicit parametrization.
- SDF representations enable **compact geometry encoding** directly from point clouds.
- The workflow **accurately predicts both integral quantities and flow fields** on unseen geometries.
- Results on the DrivAer benchmark highlight the potential of geometric deep learning for industrial CFD surrogate modeling.

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Thank you

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