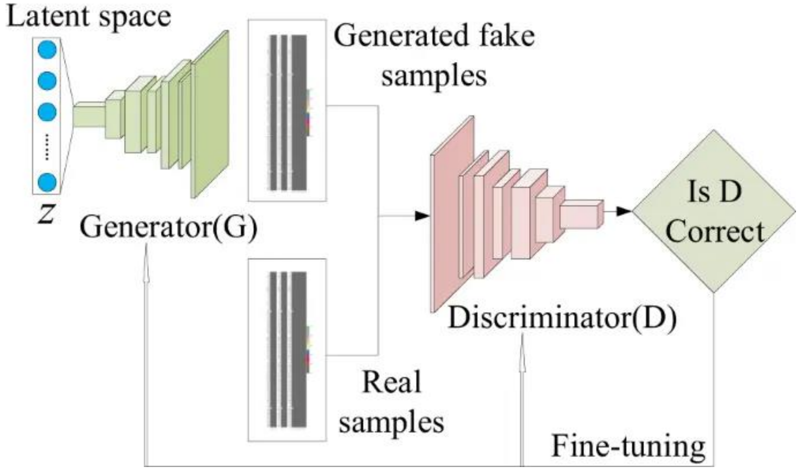
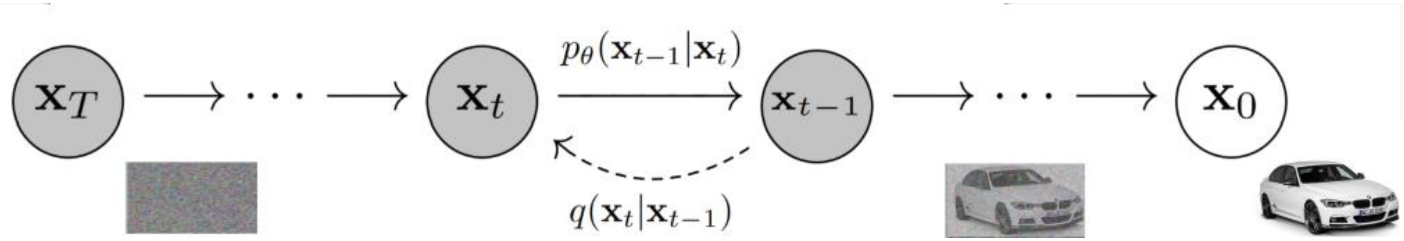
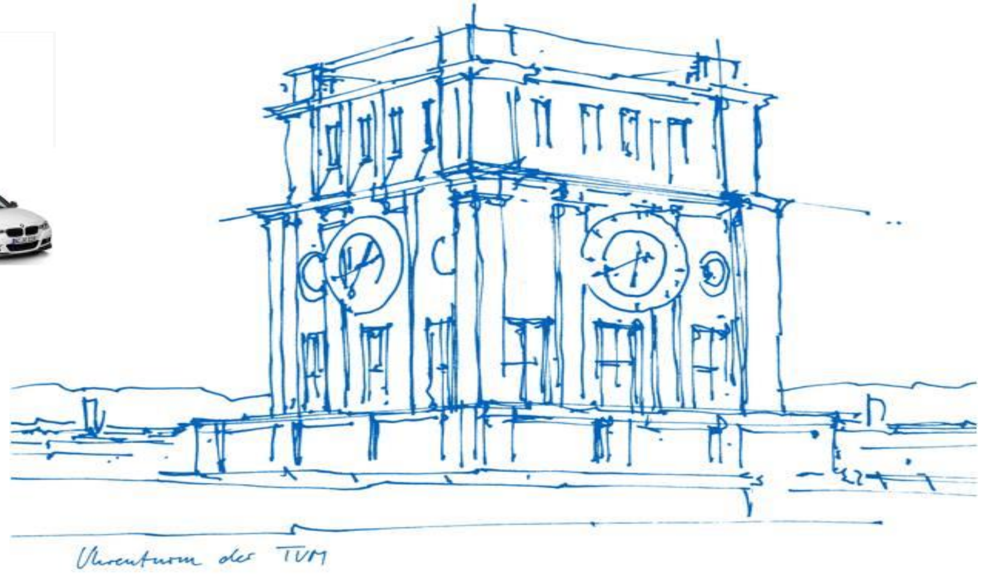


Generative AI based Geometry Generation for CFD





Master's Thesis
Kartik Bali
Advisor: Prof. Nils Thuerey
Supervisor: Dr. Babak Gholami
27.05.2024

GENERATIVE AI

- **Generative AI:** AI where DL models that learn inherent structure of input data and generate new data**.**
- **Applications:** Text content creation, Image content creation via captioning, Language translation, Video Generation, Music Generation and so many more.
- **Potential Application in Engineering Design**
  - Unexplored in areas where core engineering is involved.
  - Harness generative AI to design objects with key physical properties (optimal aerodynamic performance, structural durability, easy manufacturability).

Image to image translation via

Plug n‘ Play Diffusion by NVIDIA

GENERATIVE AI BASED DESIGN

- **Generative AI based Product Development:** Harness generative AI to come up with **aerodynamically optimal starting geometries** of car parts that are not available.
- **Easier adaptation of design variations:** Faster prototyping and engineering assessment via physical simulations.
- **Automating Initial design:** Additional agility and cost-saving in the design and production pipeline.

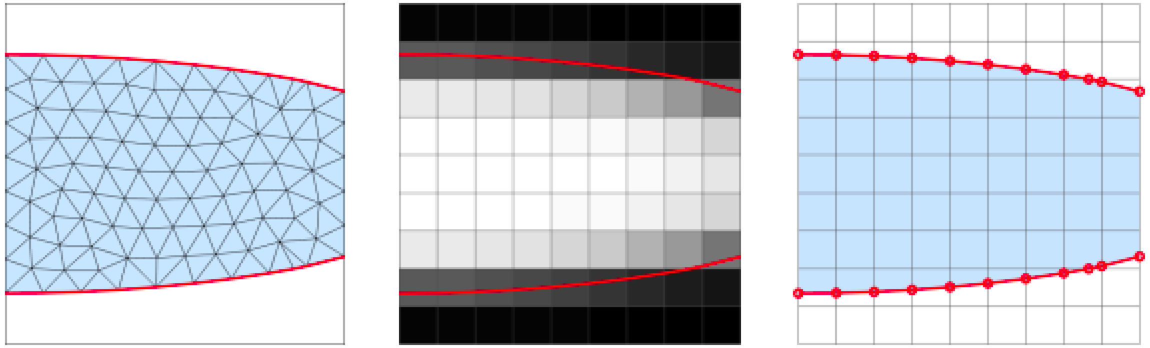
Aerodynamic Body

Spoiler and Exhaust Manifold Geometries

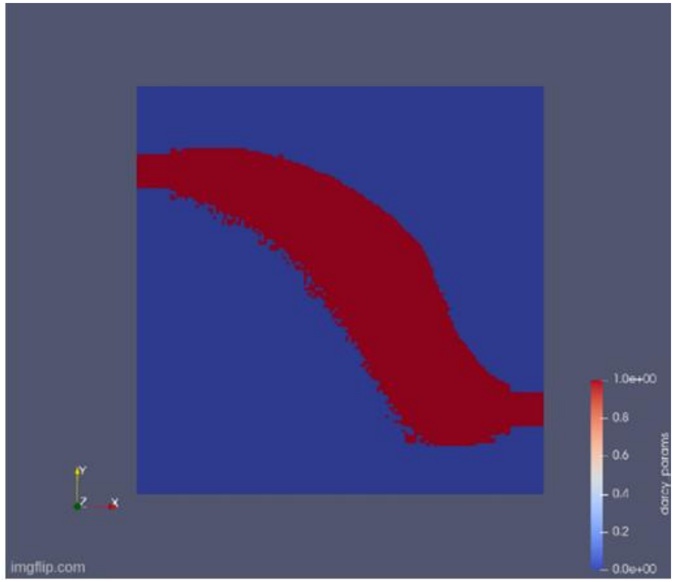
(BMW M3 GTR Featured in NFS MW 2002)

TOPOLOGY OPTIMIZATION IN CFD

- **Topology Optimization**: Optimizing material layout with the goal for maximizing an objective given certain physical constraints.
- **Why?**: Car parts must be generated in a way to minimize pressure losses for better energy efficiency. Lesser the pressure loss, lower the power required to push the fluid through.



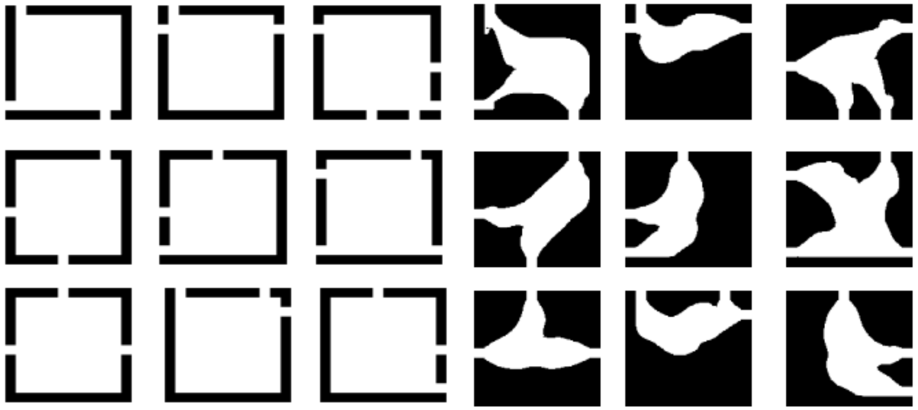
Body Fitted, Density and Level set methods for Topology Optimization



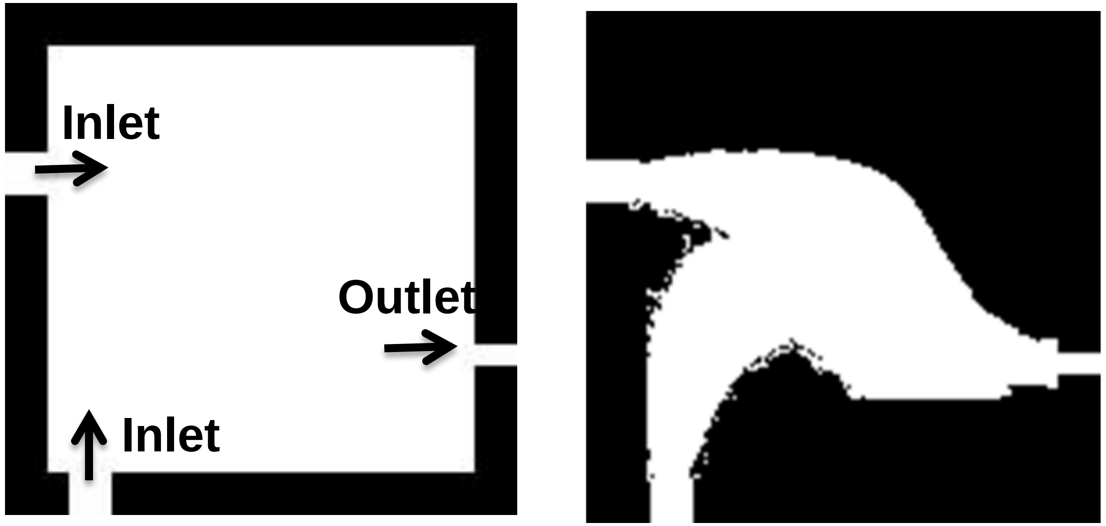
Topology Optimization of an S-bend geometry, with left inlet and right outlet

DESIGN PROBLEM-2D

- Every face of the domain: At most **2 inlets** or **1 outlet**.
- Inlets/Outlet chosen from the position set: **{2,5,9}** on each wall.
- Velocity inlet fixed to 1.0 on all inlets.
- Zero pressure boundary condition on the outlet.
- **Gen AI Aim:** Predict an optimal **starting** topology to guide the flow in a square domain



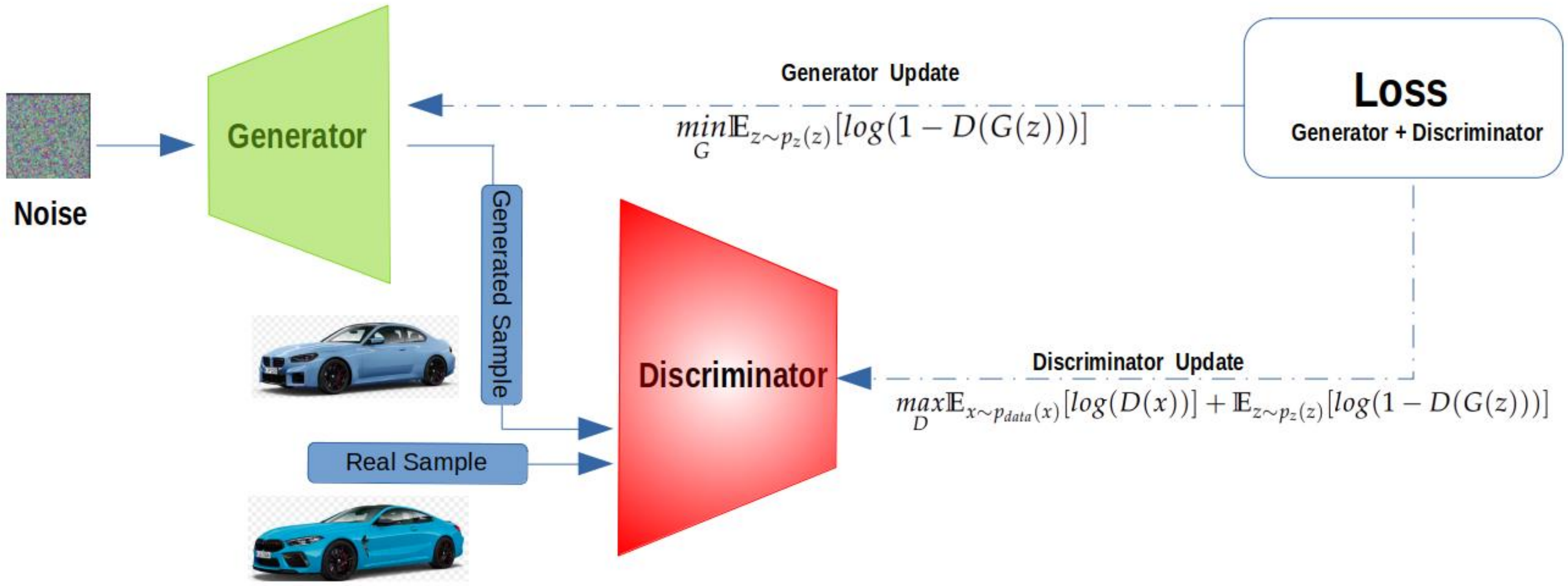
Sample Test cases generated



Initial Domain (left) and Optimized Domain (right)

GENERATIVE NETWORKS - GANS

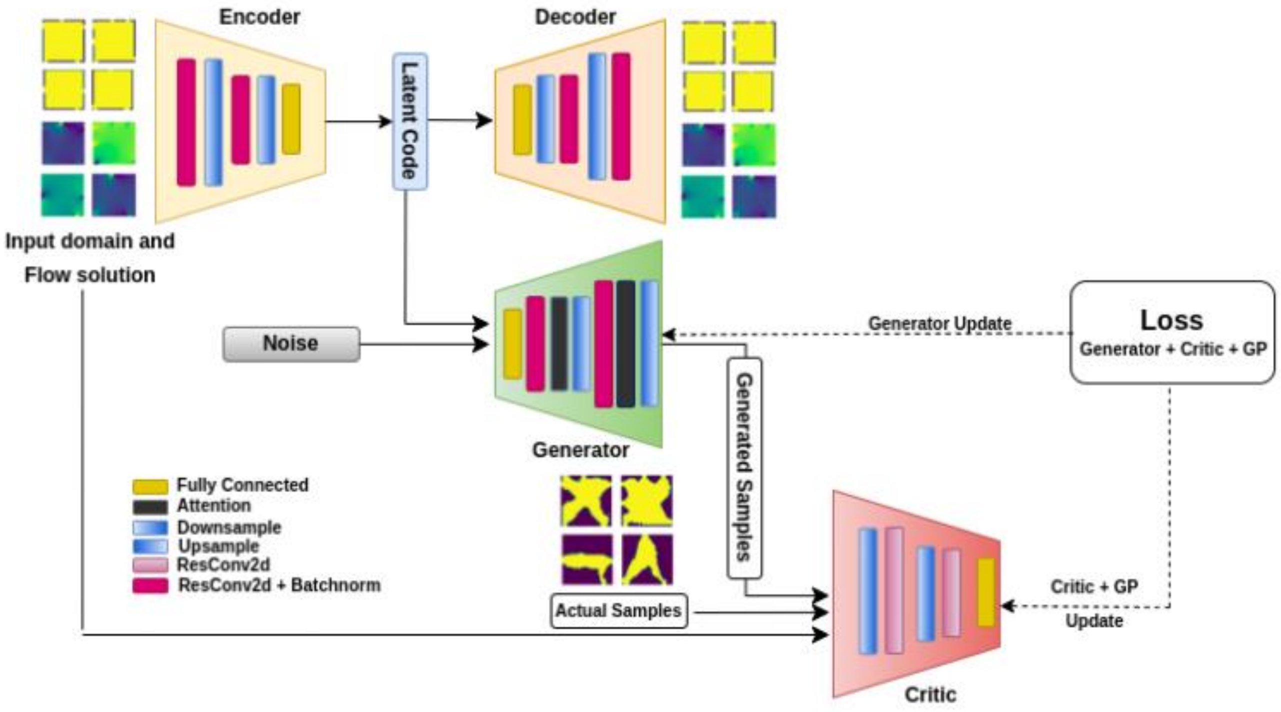
- An ideal **GAN** has a **Nash equilibrium** established between **G** and **D**.
- **G** becomes really good at predicting realistic samples, which **D** finds it considerably hard to classify from true samples**.**
- Typically ordinary **GANs** suffer from mode collapse and training instabilities.
- **Solution**: **Wasserstein GANs**



Vanilla GAN architecture

GENERATIVE NETWORKS – CONDITIONAL WGANS-GP

- **Wasserstein GANs**: Highly stable to train with no mode collapse.
- **New Loss**: Wasserstein distance between fake image and actual training image distributions.



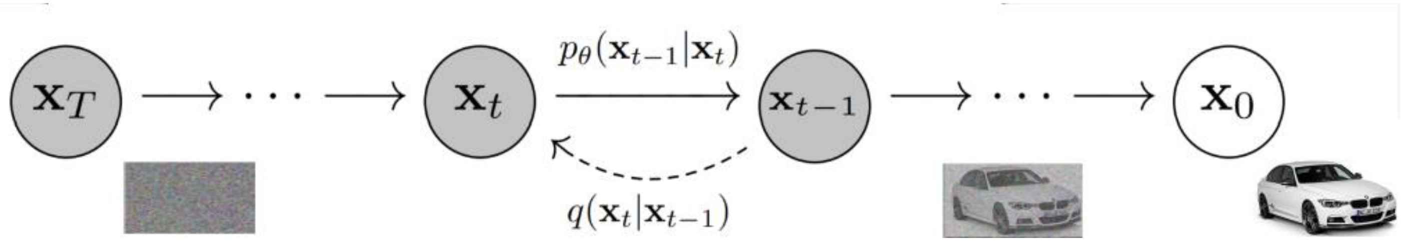
Conditional WGAN architecture

GENERATIVE NETWORKS –
DENOISING DIFFUSION PROBABILISTIC MODELS

- **Diffusion models** are the state of the art for generating high resolution image samples.
- Parametrized markov chains that gradually denoise gaussian noise to training samples.
- Use a Deep Neural Network to predict noise required to progressively denoise a sample.

$$\varepsilon_t = \varepsilon_\theta(x_t, t)$$

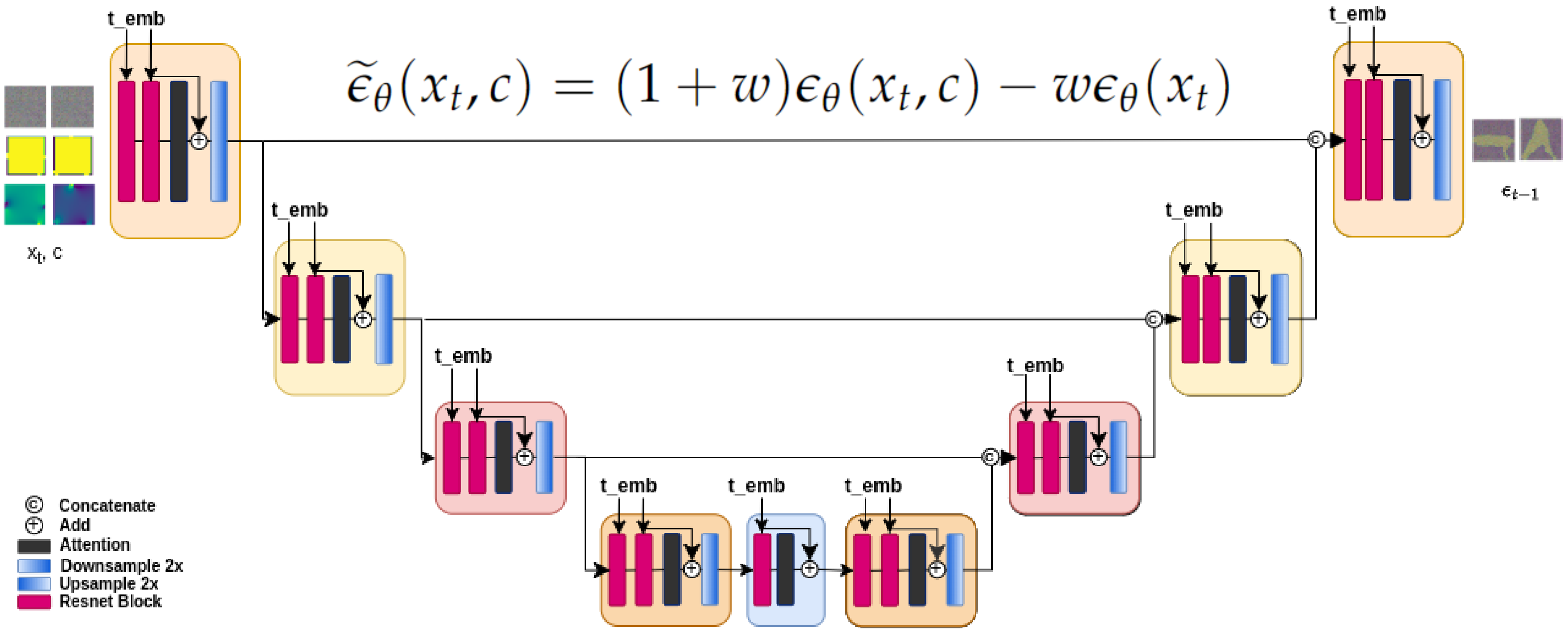
$$p_\theta(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \beta_t \mathbf{I})$$



Denoising Probabilistic Diffusion Models

GENERATIVE NETWORKS – CLASSIFIER FREE DIFFUSION MODELS

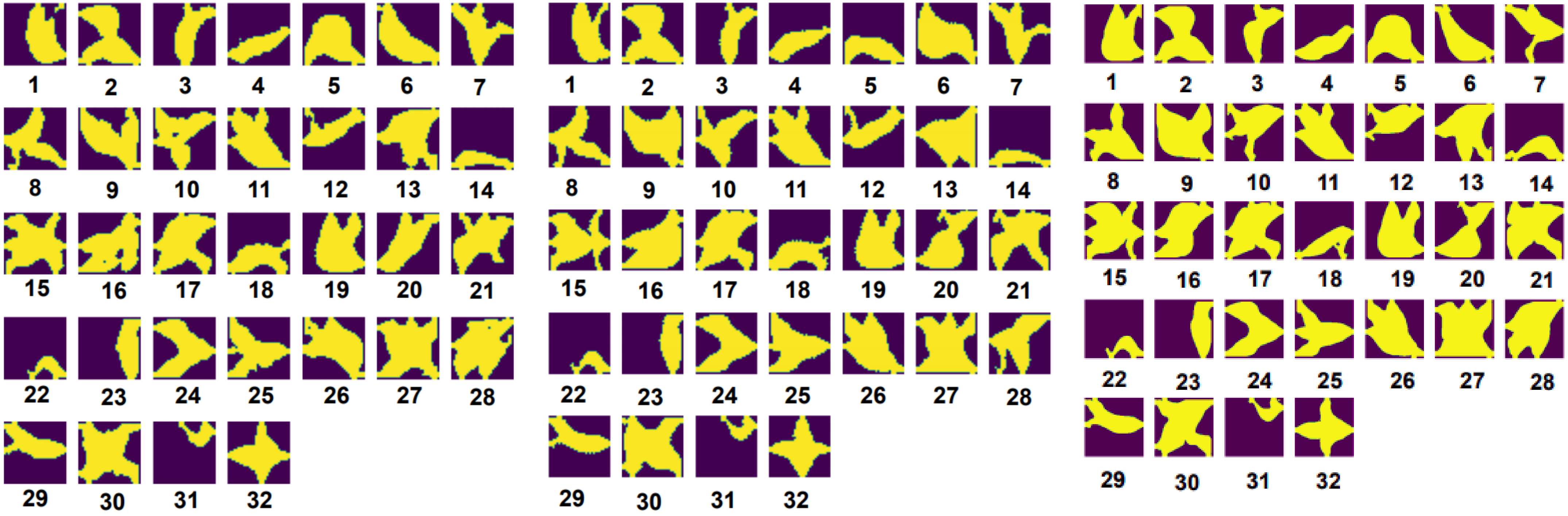
- **U-net** model as the denoising network in the diffusion model.
- To condition our diffusion model we use Classifier Free Diffusion.
- During recursive sampling we then use both conditional and unconditional versions of the denoising network.



U-net model

GENERATIVE NETWORKS – TRAINING AND INFERENCE RESULTS

- Both networks highly successful in predicting visually accurate topologies on the test set.
- Diffusion presented slightly better results than WGANs while taking more inference time ~3 times more inference time.

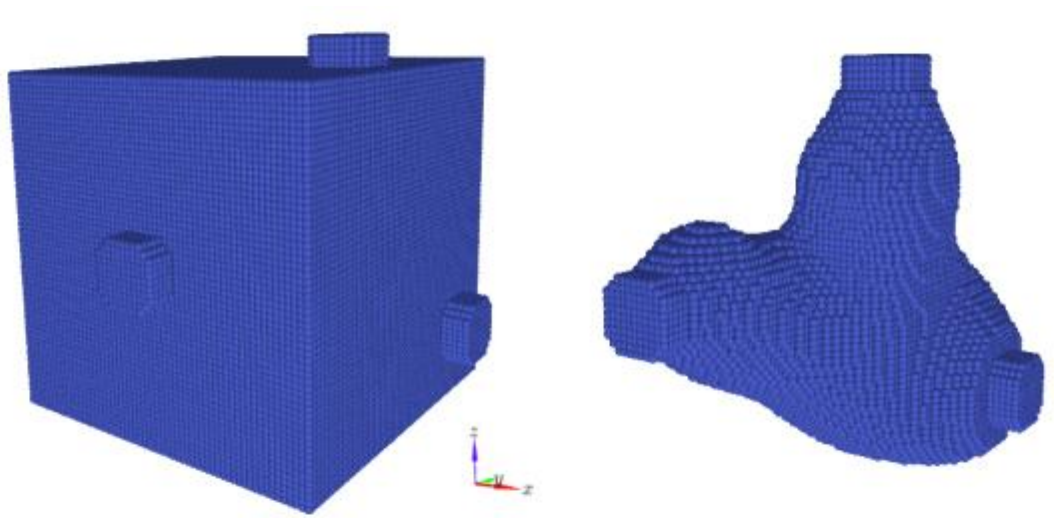


WGANs, Diffusion and Targets (left to right)

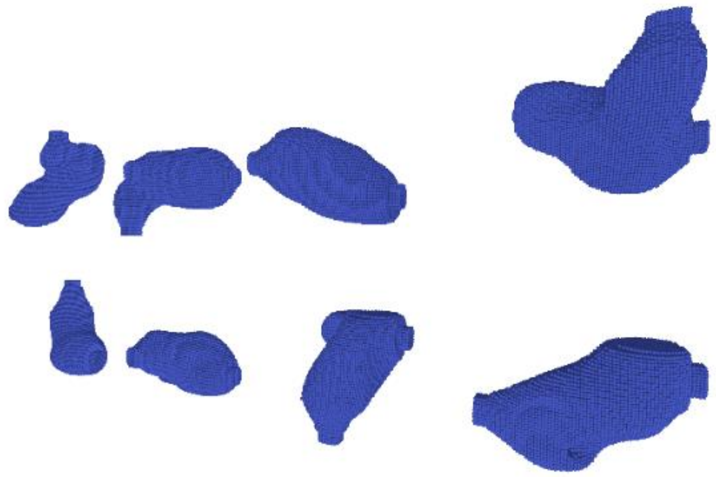
DESIGN PROBLEM – 3D

- To test our networks for prediction on 3D geometries, we extend our problem definition to 3D.
- We now optimize a design domain of 64X64X64 cells, and compute flow optimal topologies in a cubical domain.

$$(x,y)_{orifice} = \{(\alpha,\beta) | \alpha \in \{2,5,8\}, \beta \in \{2,5,8\}\}$$



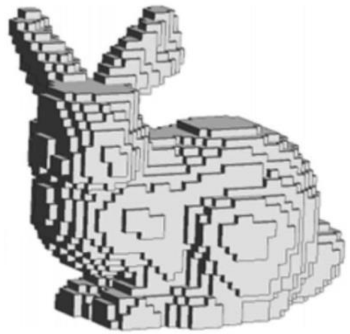
Initial domain (right) and optimal domain(left)



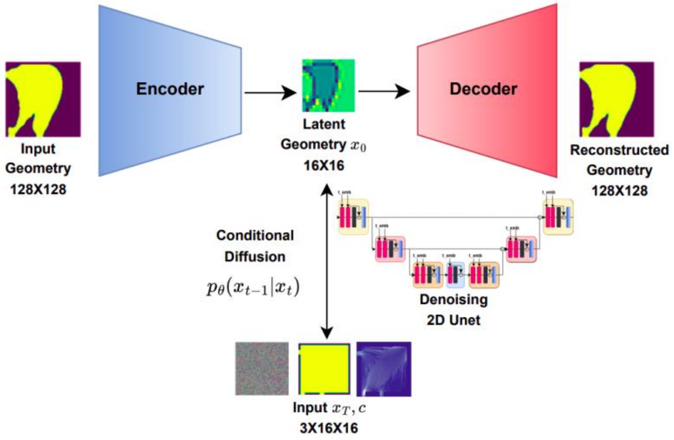
Example training samples generated

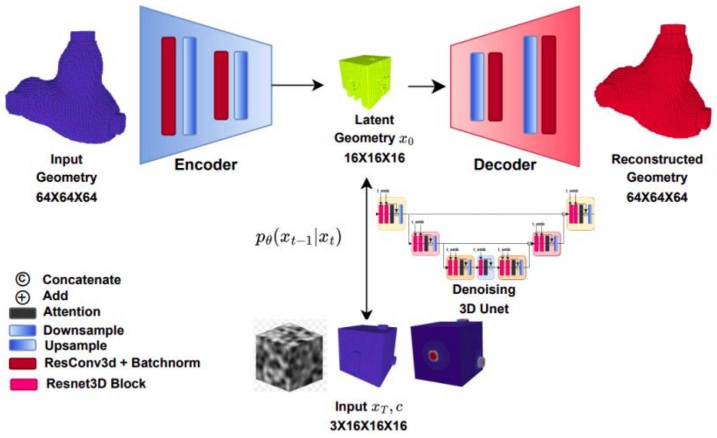
GENERATIVE NETWORKS – LATENT DIFFUSION

- Even reasonable voxel geometries (here **64X64X64**) consume a lot of memory while training for reasonable batch sizes.
- To counter this -> **Diffusion on low resolution latents** that are easy to store and train generated by an **Encoder**
- Pass the **denoised latents** through a **Decoder** for **super-resolution**.



Stanford Voxel Bunny

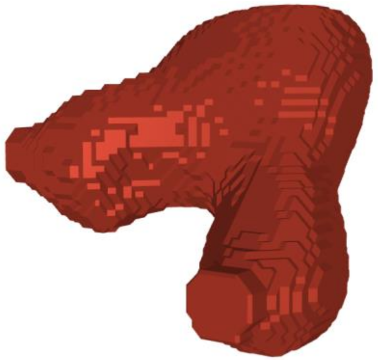




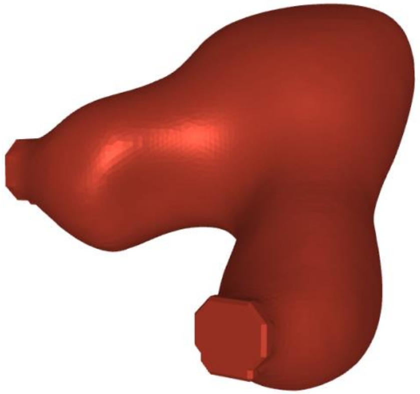
Latent Diffusion Models for 2D and 3D geometry generation

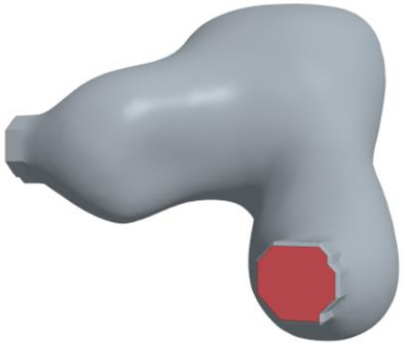
MAIN GOAL: PREDICTION OF OPTIMAL STARTING GEOMETRIES

Design Inputs → **Starting Geometry** (via Generative AI/ Topology Optimization) → **Smoothing** → **Shape Optimization** → Further Processing ... → **Final Design Geometry**



Our Solution





POST PROCESSING

- Another important objective of this work is to synthesize geometries that could provided for further analysis at BMW in form of CAD models.
- **Predicted geometries**: Converted to **mesh** from **voxel** representations using **Marching Cubes**, and then smoothened using multiple rounds of laplacian smoothing.

Conversion of Voxel geometry to Mesh to Smooth Mesh

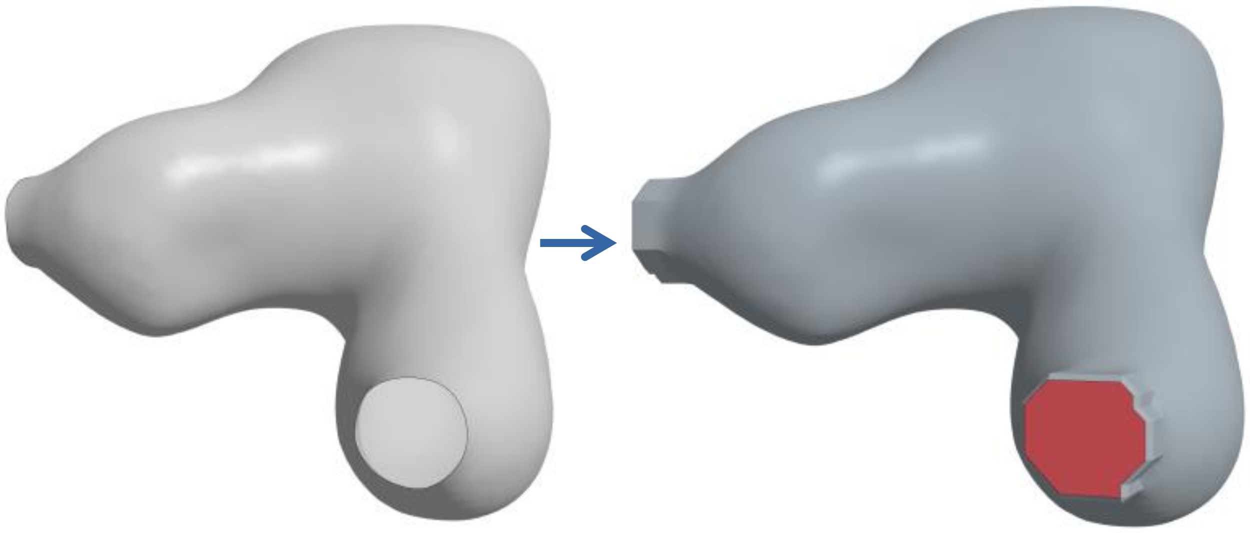
POST PROCESSING

- STL format was used to convert the obtained smoothened mesh representation to usable CAD surface geometry file..
- Needed to seclude the inlet and outlet faces from the rest of the geometry to set boundary conditions.

solid name
  facet normal $n_i\ n_j\ n_k$
    outerloop
      vertex $v1_x\ v1_y\ v1_z$
      vertex $v2_x\ v2_y\ v2_z$
      vertex $v3_x\ v3_y\ v3_z$
    endloop
  endfacet
endsolid

Total faces in solid

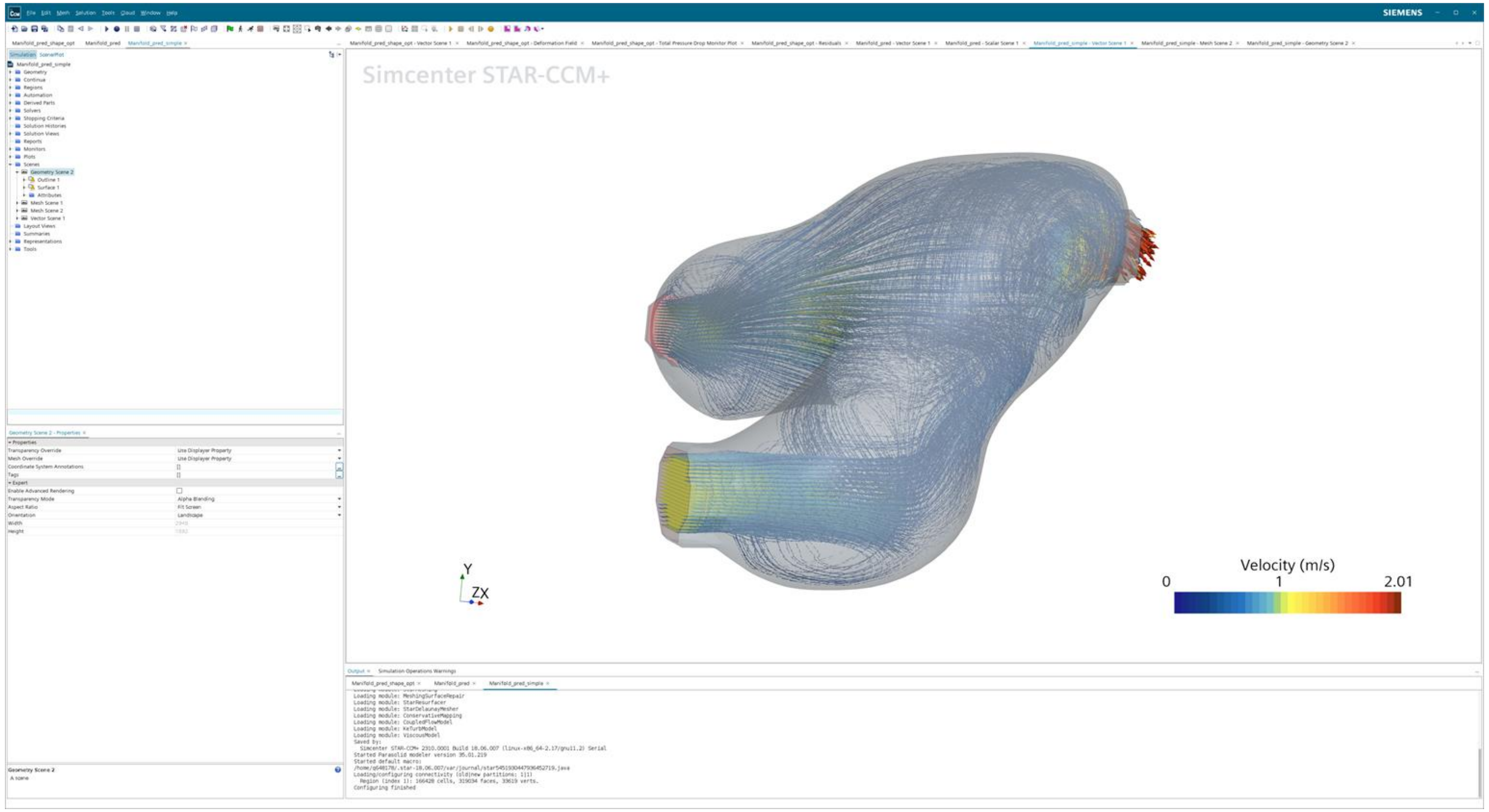
STL format



Conversion of Raw mesh to STL format

POST PROCESSING

- After setting up the boundary conditions, the geometries could then be simulated in StarCCM+, via a simple surface import and setting appropriate flow model and boundary conditions.



Flow Streamlines on the generated geometry after successfully import in StarCCM

CONCLUSION AND FUTURE WORK

- This work shows that generative AI is highly capable of accelerating and providing geometries that obey design considerations.
- This work directly produces STL format geometries that could be handed over for flow based analysis at BMW.
- While Phiflow is highly customizable and fast, it still has limited capacity for topology optimization:
- In future better optimization tools could be used to automate generation of variety of other test cases.
- Next Step in Generative Design (smoother geometry generation):
  - **Differentiable geometry generation : Representations like NURBS (Non Uniform Radial B-Spline) and Diffusion Maps**
  - **Faster ML inspired solvers to guide generation through physics**

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