Generating near-optimal meshes using green AI

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Outline

- Motivation – The carbon footprint of HPC
- Our AI systems to predict mesh spacing using
  - Mesh sources
  - Background meshes
- Examples
- How green is the AI system?
- Concluding remarks

The carbon footprint of HPC

THE MIT PRESS READER

"The Cloud now has a greater carbon footprint than the airline industry. A single data centre can consume th ... es."

HPC wire

"The Exascale era is here and po... consumption for HPC is skyrocke..."

ICTFOOTPRINT.EU

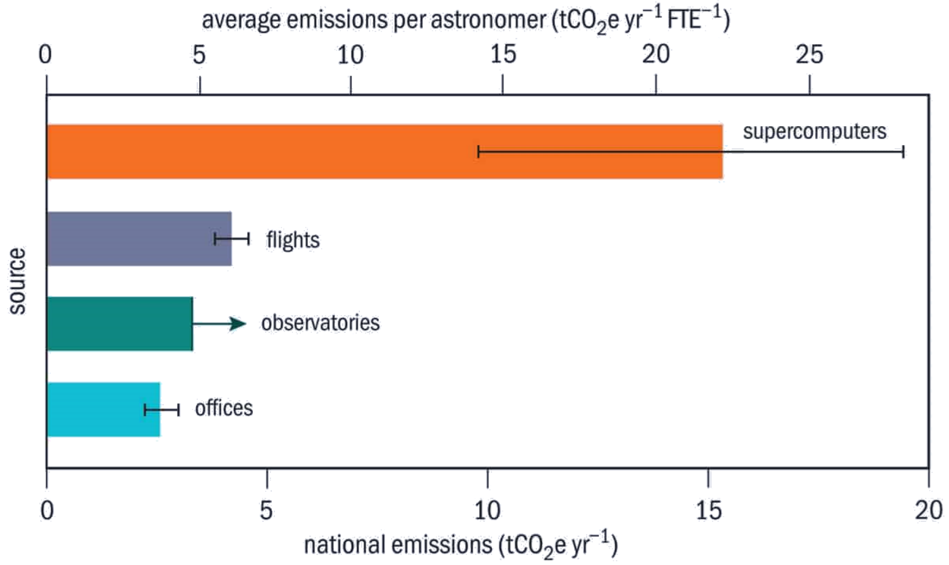
BMW Group moves HPC to Iceland to reduce CO_2 by 3.5K tC02/year

bcs The Chartered Institute for IT

"Carbon footprint, the (not so) hidden cost of HPC."

IOP Publishing

The huge carbon footprint of large-scale computing



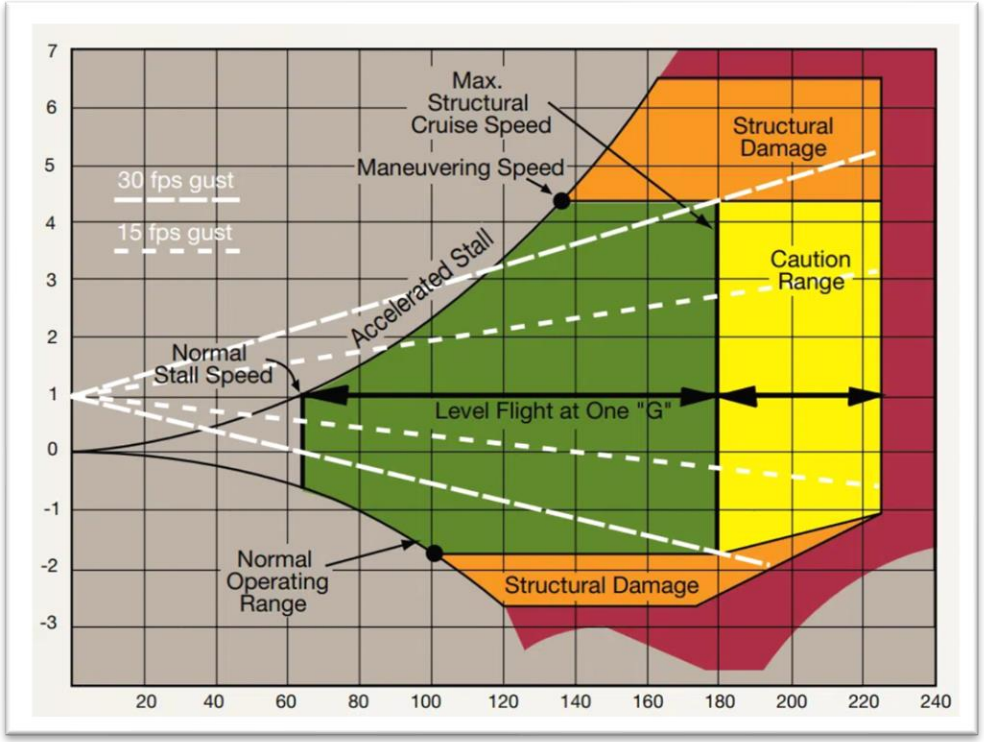
ASIAN SCIENTIST

Powering the world's top 500 supercomputers pumps around 2M tCO_2/year

The carbon footprint of HPC

CFD for the design of an aircraft

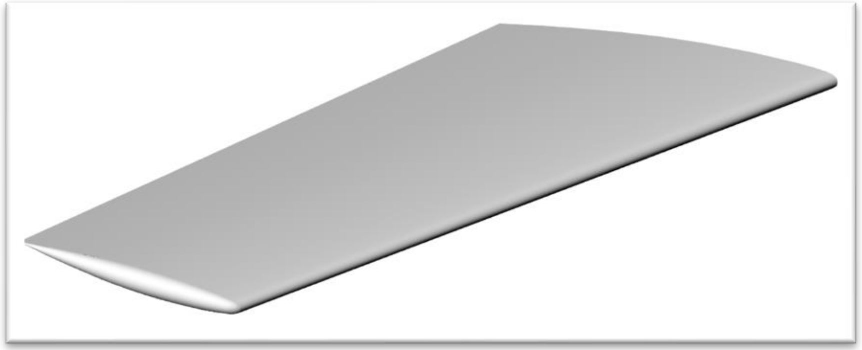
- At least 200 runs to cover the flight envelope
- Each run using ~100M elements
  (12h using 512 CPU processors)
- 1.7 T CO_2e to perform 200 runs
  - 15.5 MWh
  - 9,840 Km in a passenger car



- NASA estimates that, by 2030, simulations with ~20B elements will be commonplace
- 150 T CO_2e to perform 200 runs
  - 1,350 MWh
  - 858,000 Km in a passenger car (~20 times around the world!)

The carbon footprint of HPC

- From the point of view of simulation efficiency, each operating condition requires a different mesh



(a) $M_\infty = 0.41, \alpha = 8.90^\circ$ (b) $M_\infty = 0.79, \alpha = 5.39^\circ$ (c) $M_\infty = 0.80, \alpha = 8.19^\circ$

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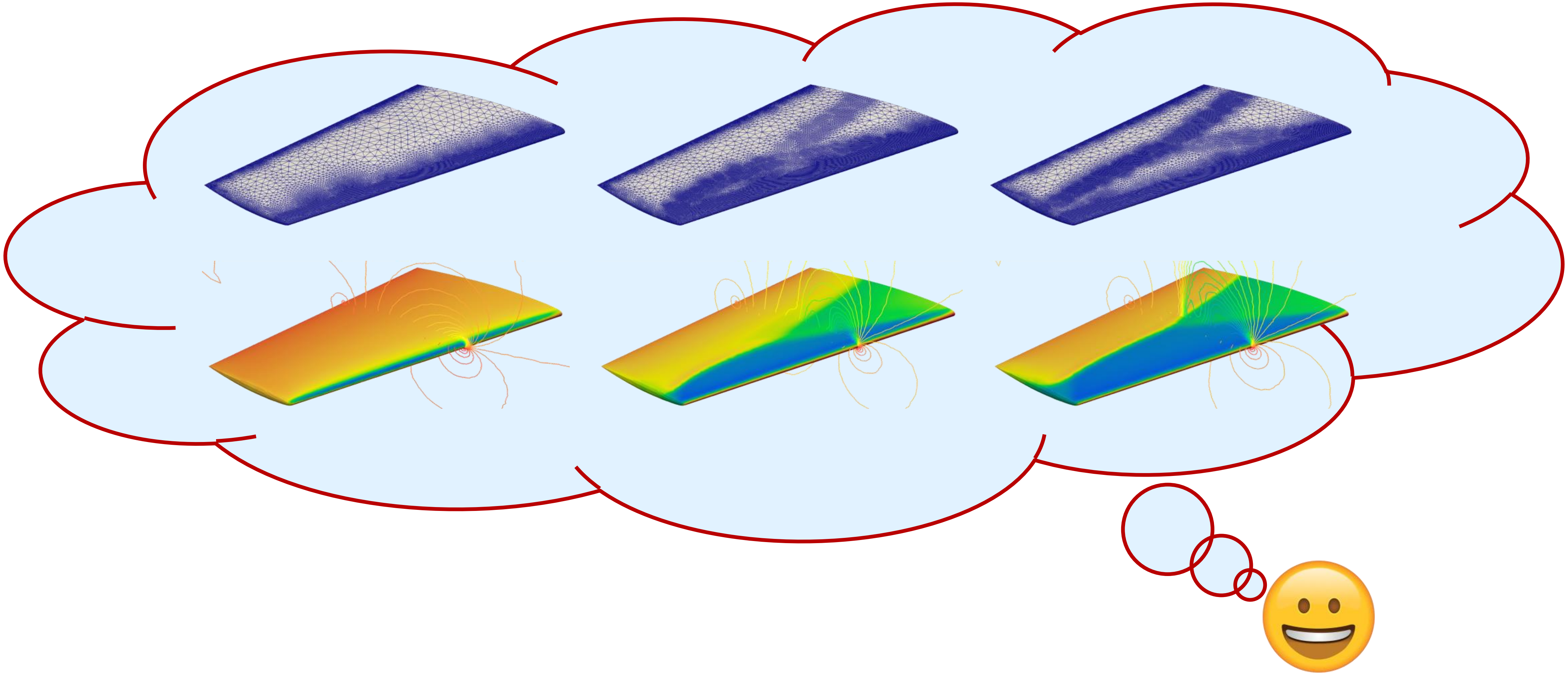
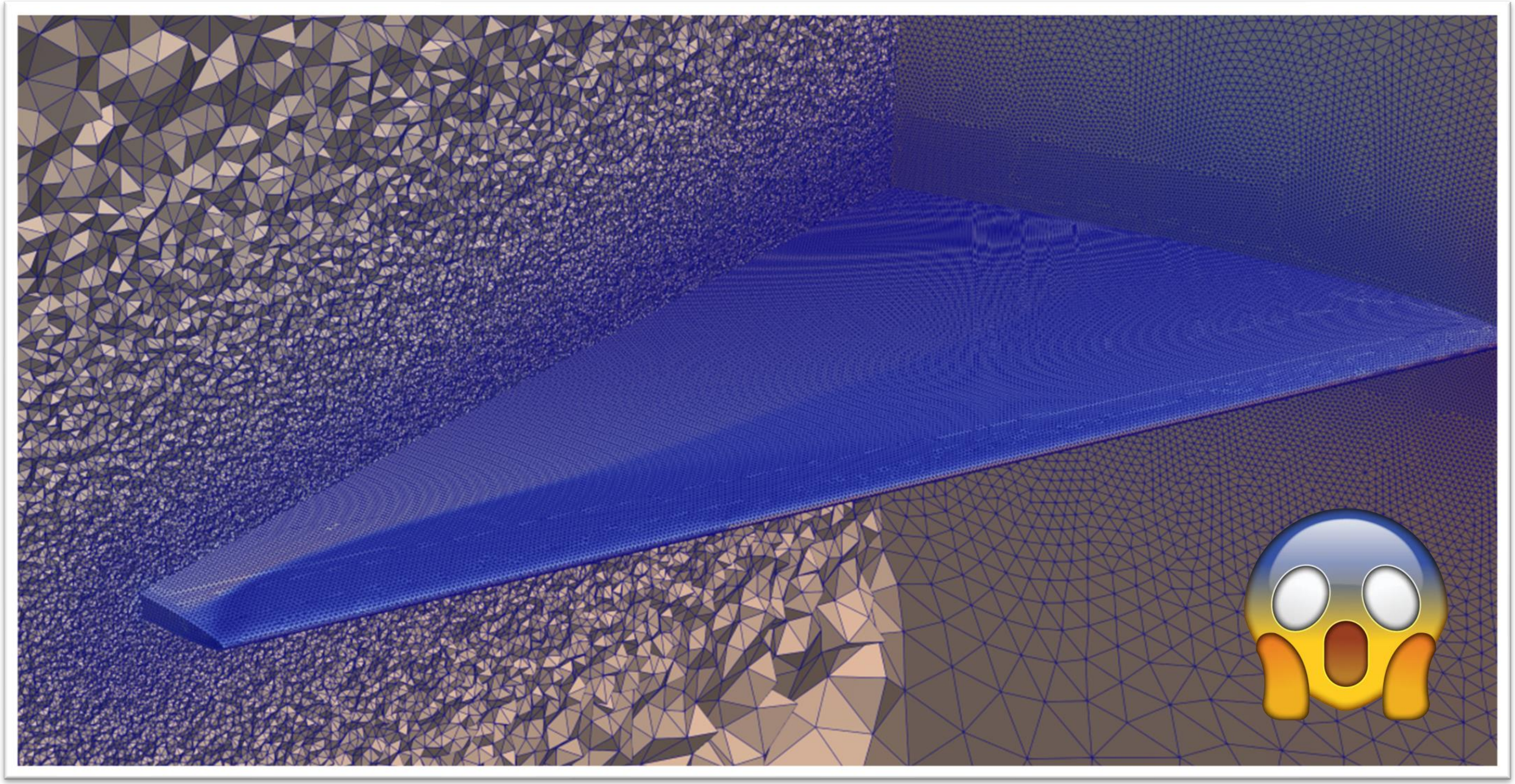


The carbon footprint of HPC

- But current industrial practice involves using over-refined meshes to avoid the requirements of human expertise and the time-consuming process of tailoring meshes



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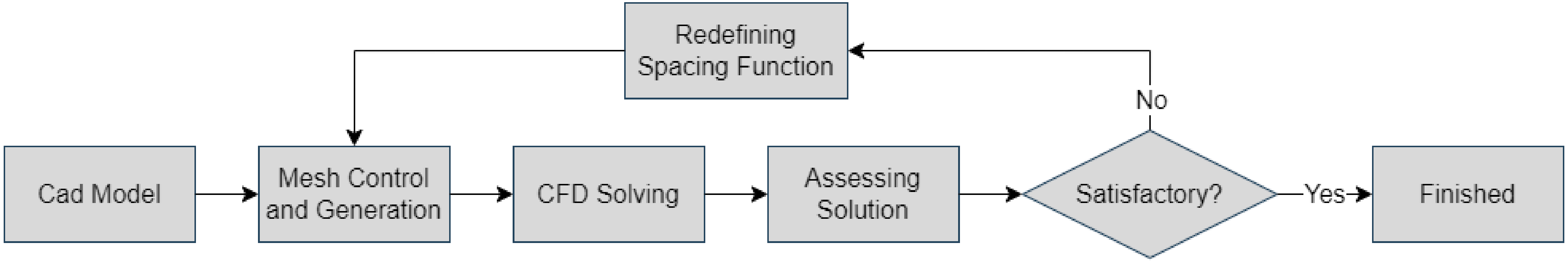
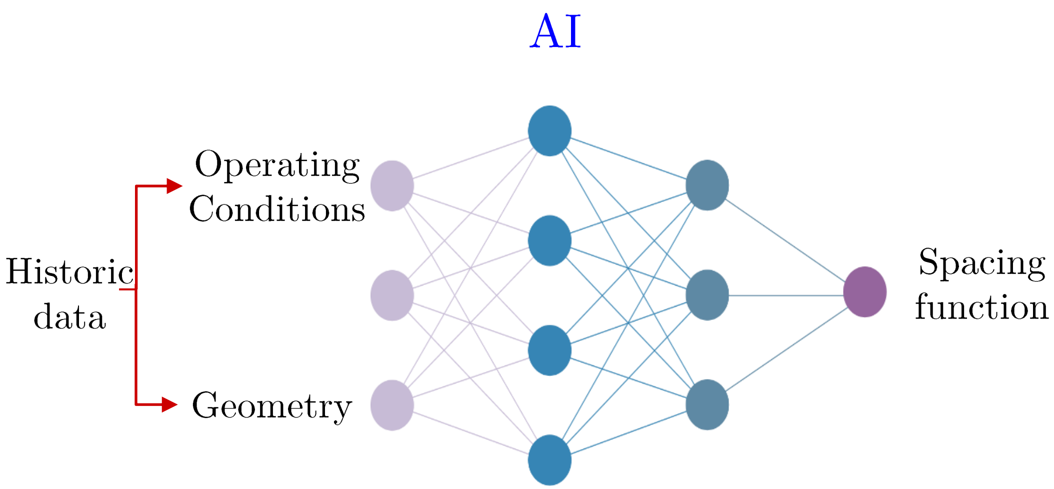
AI system to predict mesh spacing

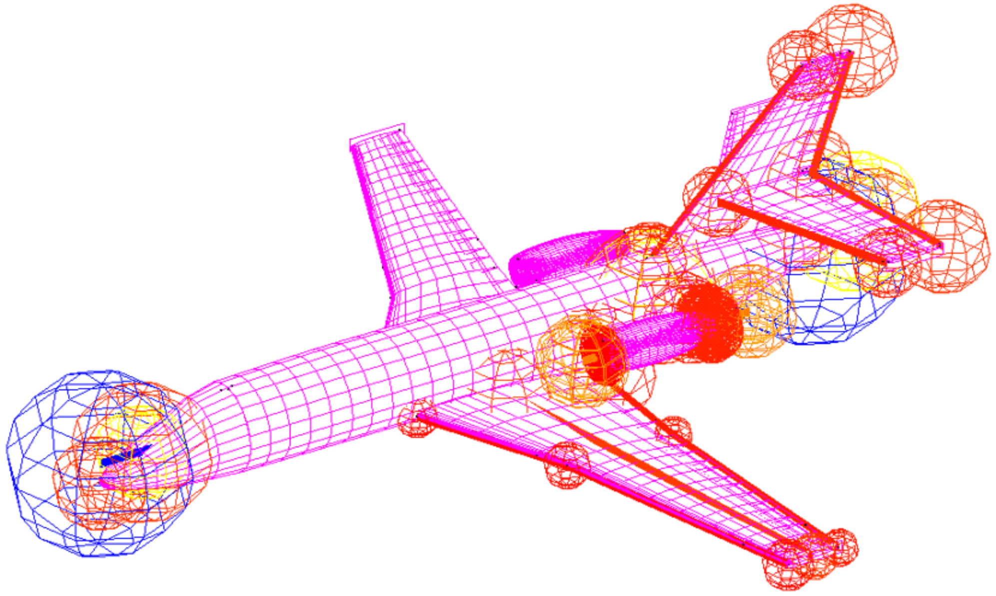


- Develop an AI capable of speeding up and automating the mesh generation process
- Accelerate mesh independent solution and speeding up the design process
- Preserving and utilising previous learnt knowledge



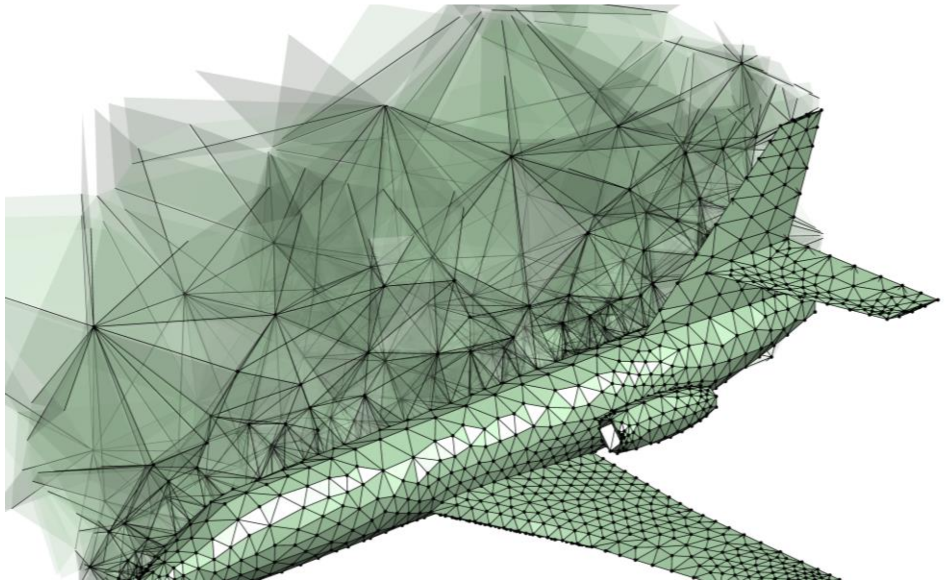
AI system to predict mesh spacing

- How is a spacing function usually defined?



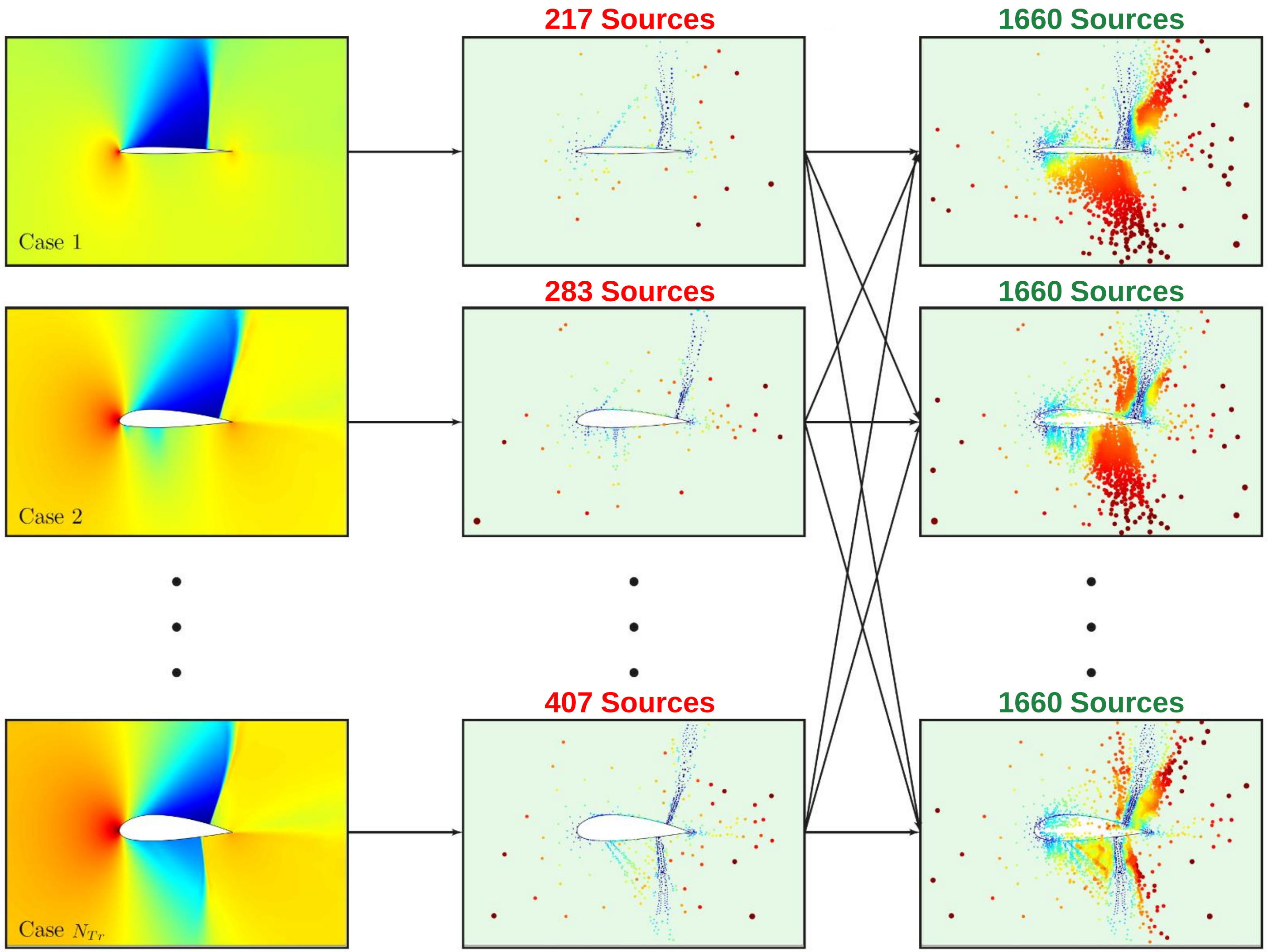
- Mesh sources (point, lines, planes, etc)
  - A point source is defined by a position, a desired spacing and a radius of influence
  - The spacing at any point is calculated as the minimum spacing defined by all the sources

- Background mesh
  - A (discrete) nodal spacing function is given
  - The spacing at any point is interpolated from the nodal spacing function in the (coarse) background mesh



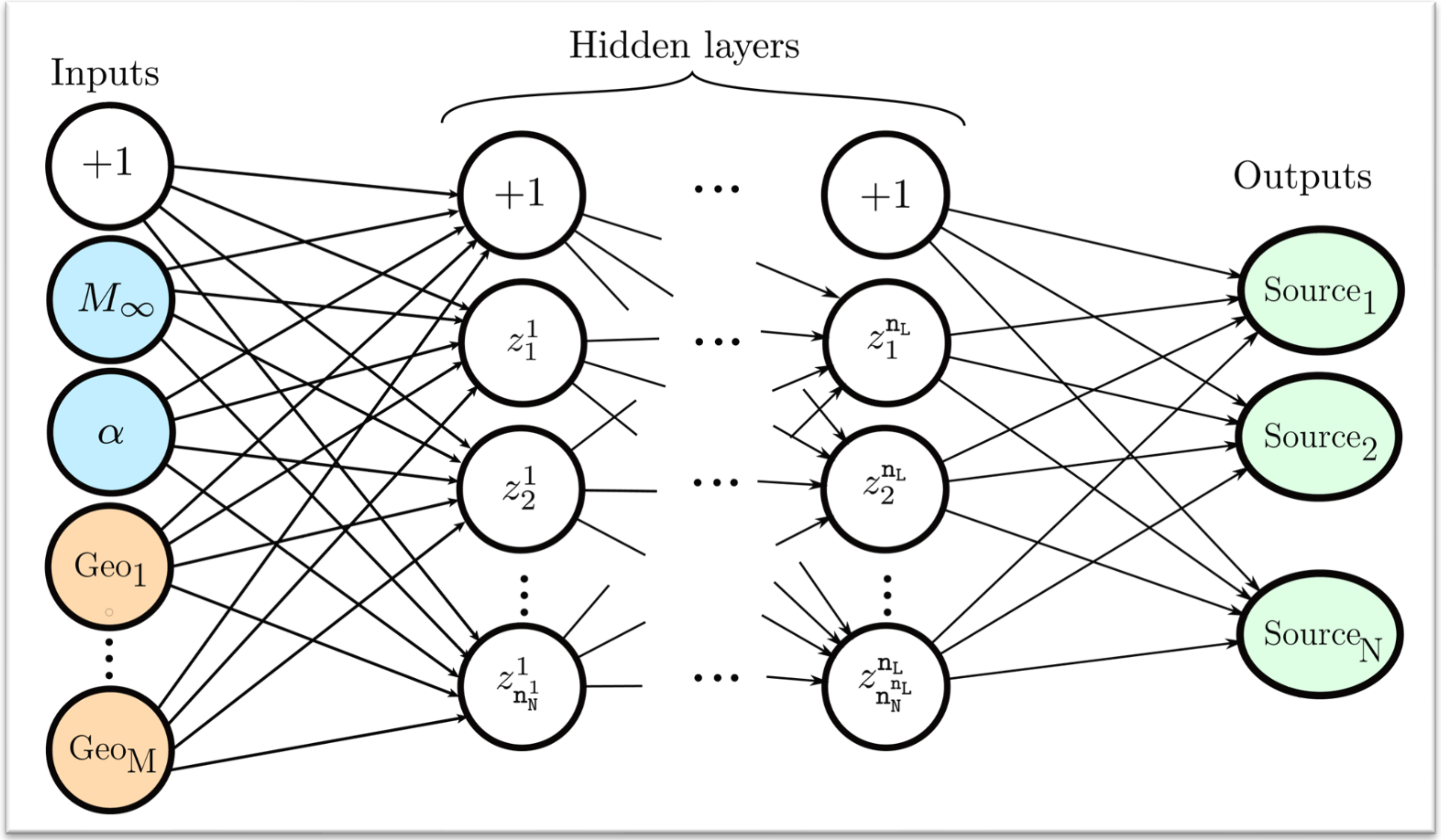
AI system to predict mesh spacing (using sources)

- Step 1 – Generate point sources from a given solution
- Step 2 – Generate global sources from sets of local sources



AI system to predict mesh spacing (using sources)

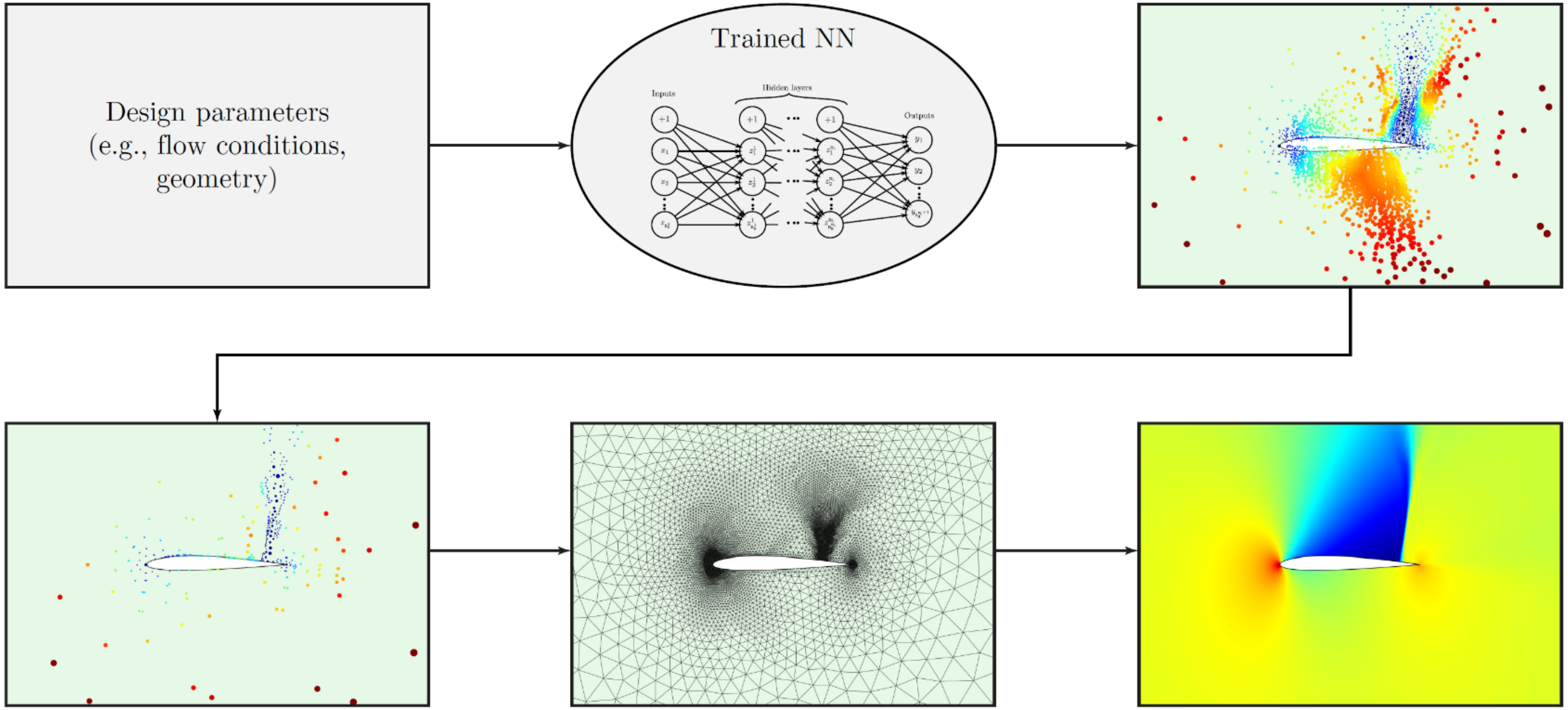
- Neural network architecture



- Each output involves a position (3 coordinates), a spacing and a radius of influence.

AI system to predict mesh spacing (using sources)

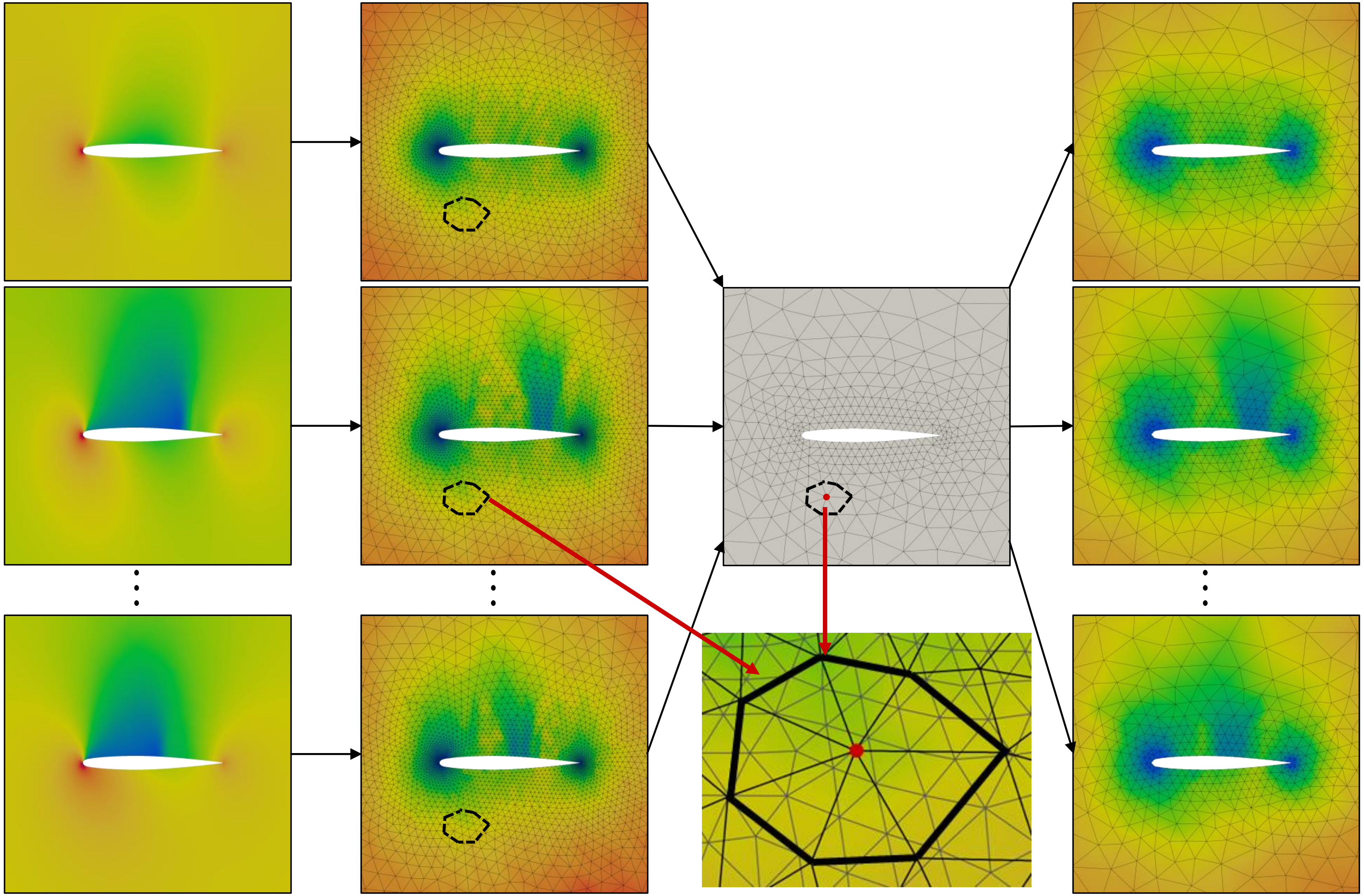
- Step 3 – Use the trained NN to predict the sources characteristics
- Step 4 – Reduce the global set of sources



C Lock, O Hassan, RS, J Jones, Meshing using neural networks for improving the efficiency of computer modelling, Engineering with Computers, 2023

AI system to predict mesh spacing (using a background mesh)

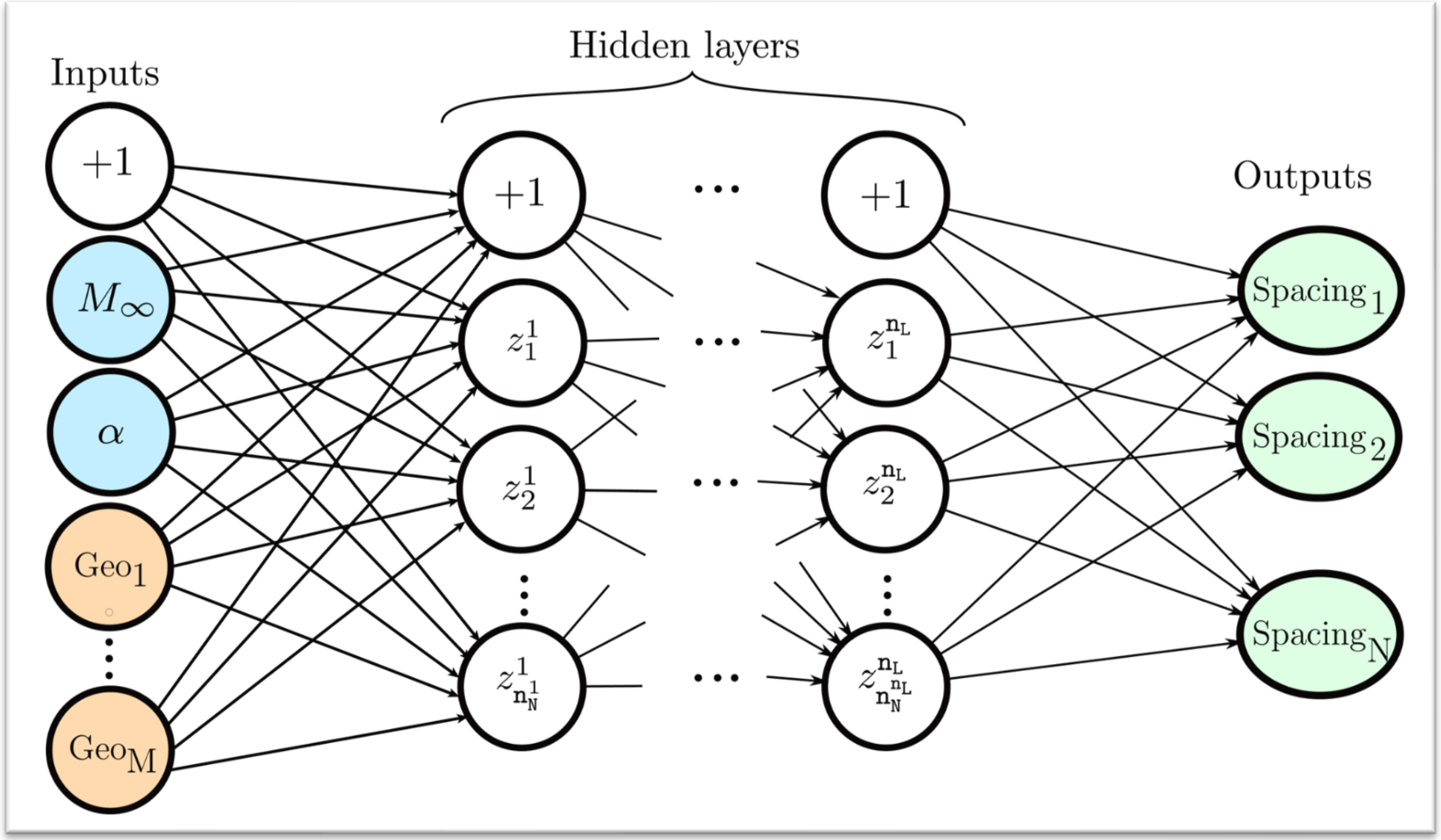
- Generate a spacing function from a given solution
- Interpolate the spacing onto a background mesh
- Take a conservative approach to interpolation



C Lock, O Hassan, RS, J Jones, Predicting the near-optimal mesh spacing for a simulation using machine learning, IMR, 2023

AI system to predict mesh spacing (using a background mesh)

- Neural network architecture



- Each output involves a spacing
- It requires mesh morphing for variable geometric configurations

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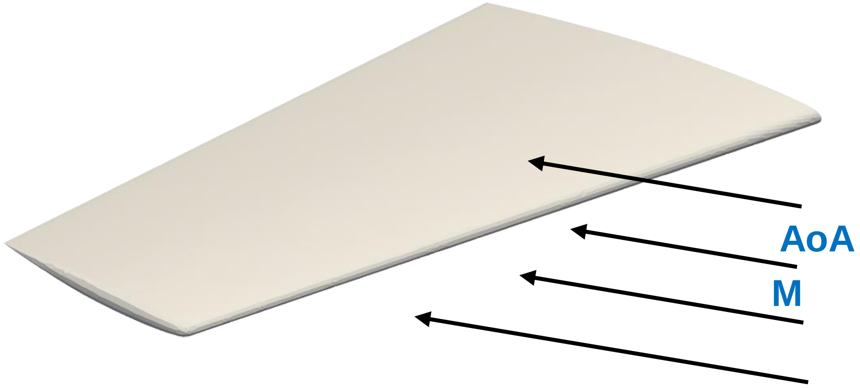
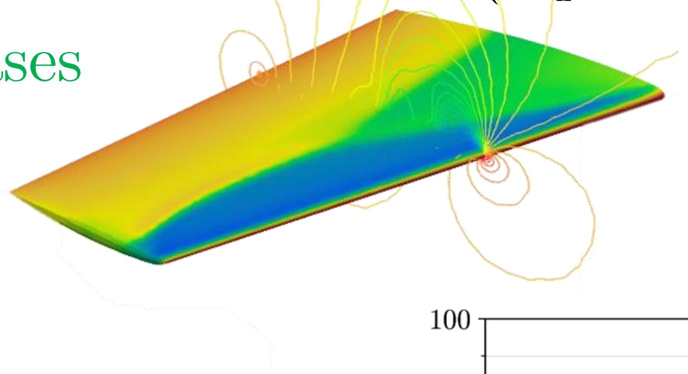
Examples

- ONERA M6 wing – Variable flow conditions
  - Mach [0.3, 0.9]
  - Angle of Attack [0, 12]
- Solution from an inviscid compressible flow solver
- 10, 20, 40, 80, 120, 160 training cases, with 100 test cases
- Hyperparameters are tuned
  - Number of hidden layers – 1, 2,…,6
  - Neurons per layer – 25, 50, 75, …, 200, 225, 250
- Using sources
  - 19,345 global point sources
- Using background mesh
  - 14,179 nodes

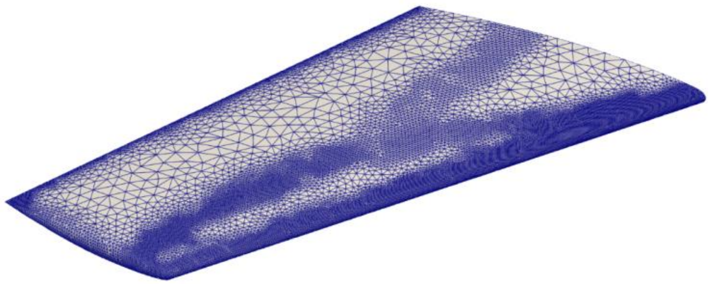


Examples

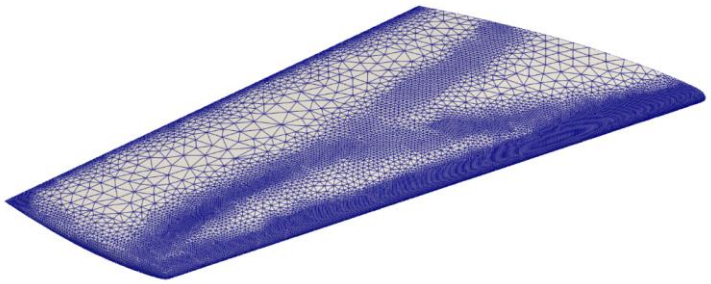
- ONERA M6 wing – Variable flow conditions (2 parameters) – 160 training cases
- Prediction for unseen test cases
  - M=0.79, AoA=5.39°



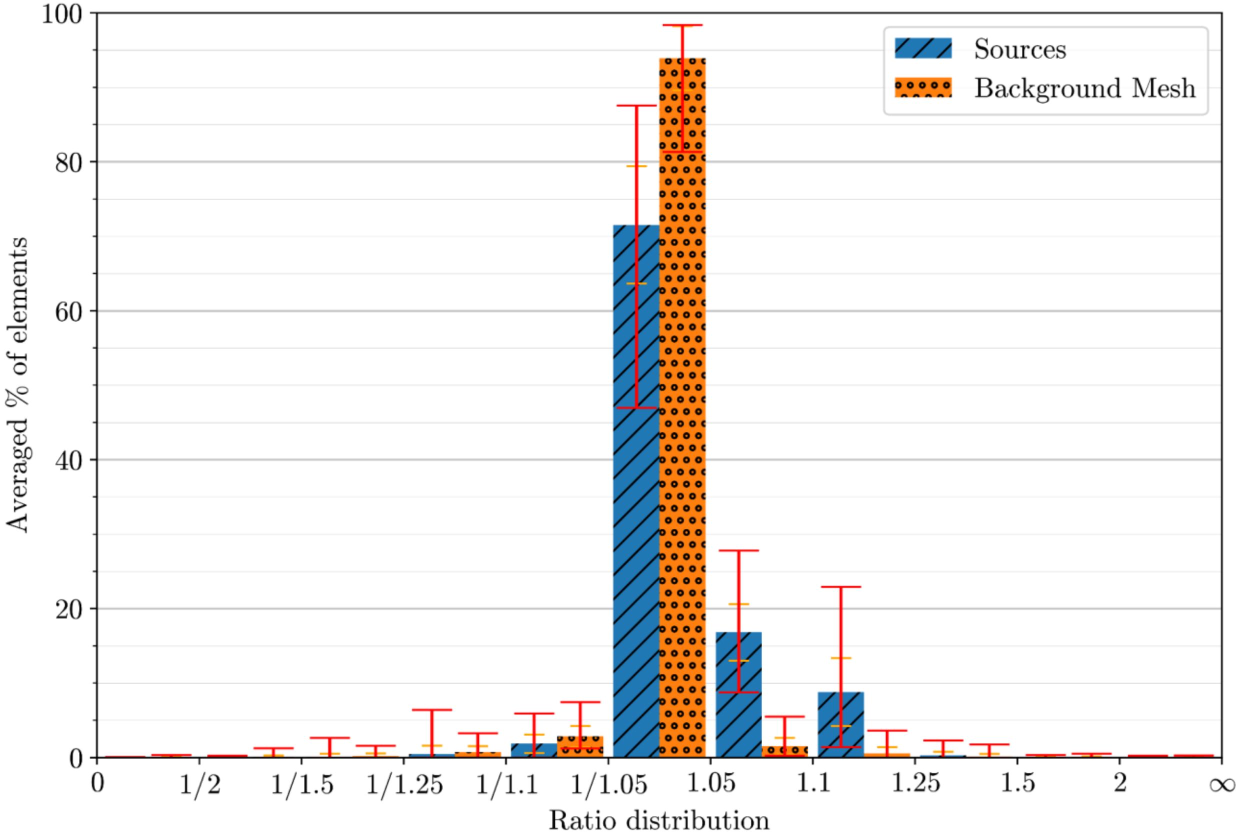
Target



ML Prediction

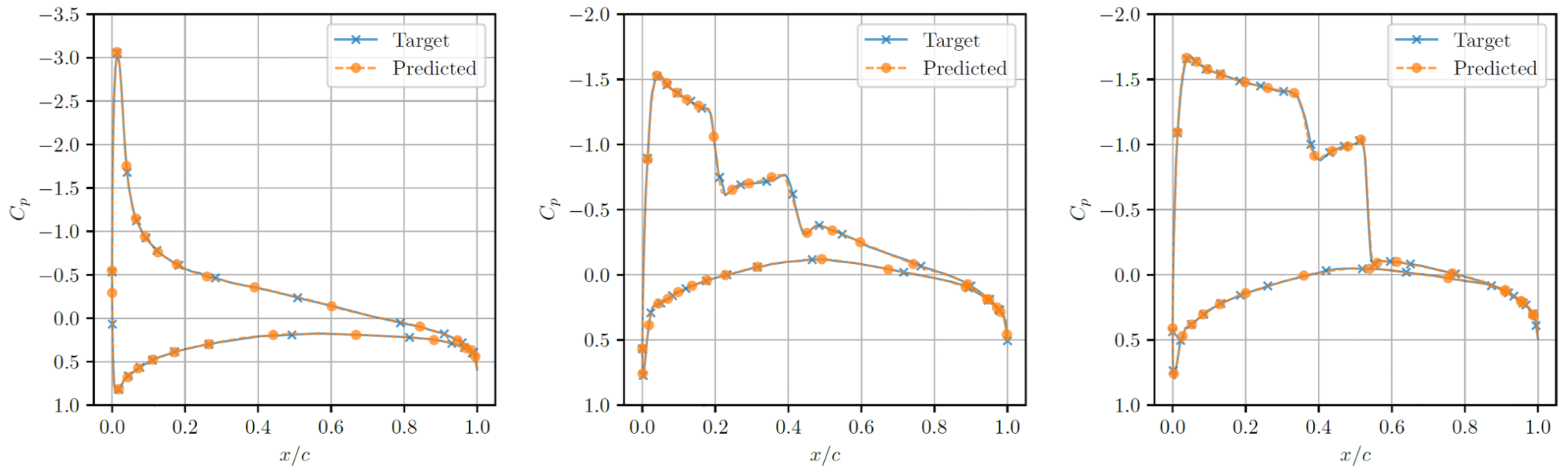


- Using sources, the spacing at 72% of the points are predicted within 5% of the target
- Using a background mesh, the spacing at 94% of the points are predicted within 5% of the target



Examples

- ONERA M6 wing – Variable flow conditions (2 parameters) – 160 training cases
- Suitability of predicted meshes to perform simulations



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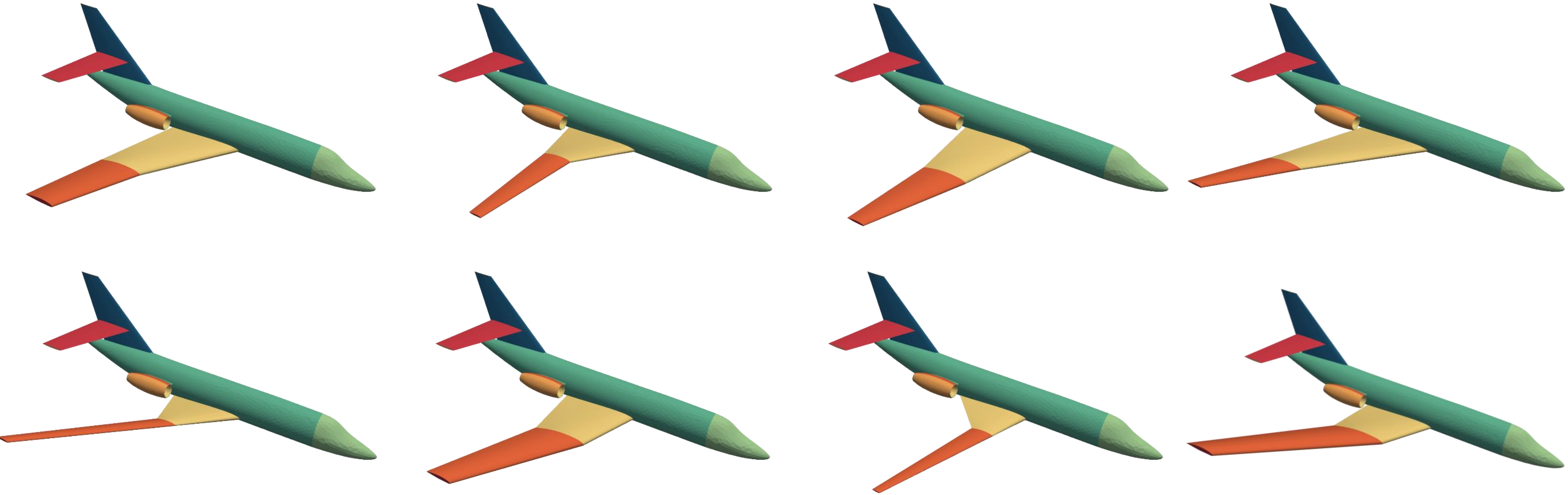
	Target	Prediction	Target	Prediction	Target	Prediction
C_L	0.605	0.603	0.469	0.468	0.722	0.723
C_D	0.0342	0.0340	0.0289	0.0287	0.0828	0.0828

Examples

- Full aircraft – Variable geometry (11 parameters)
  - Spacing prediction using a background mesh
  - Flow conditions – M=0.8, AoA=2^{o}



Examples

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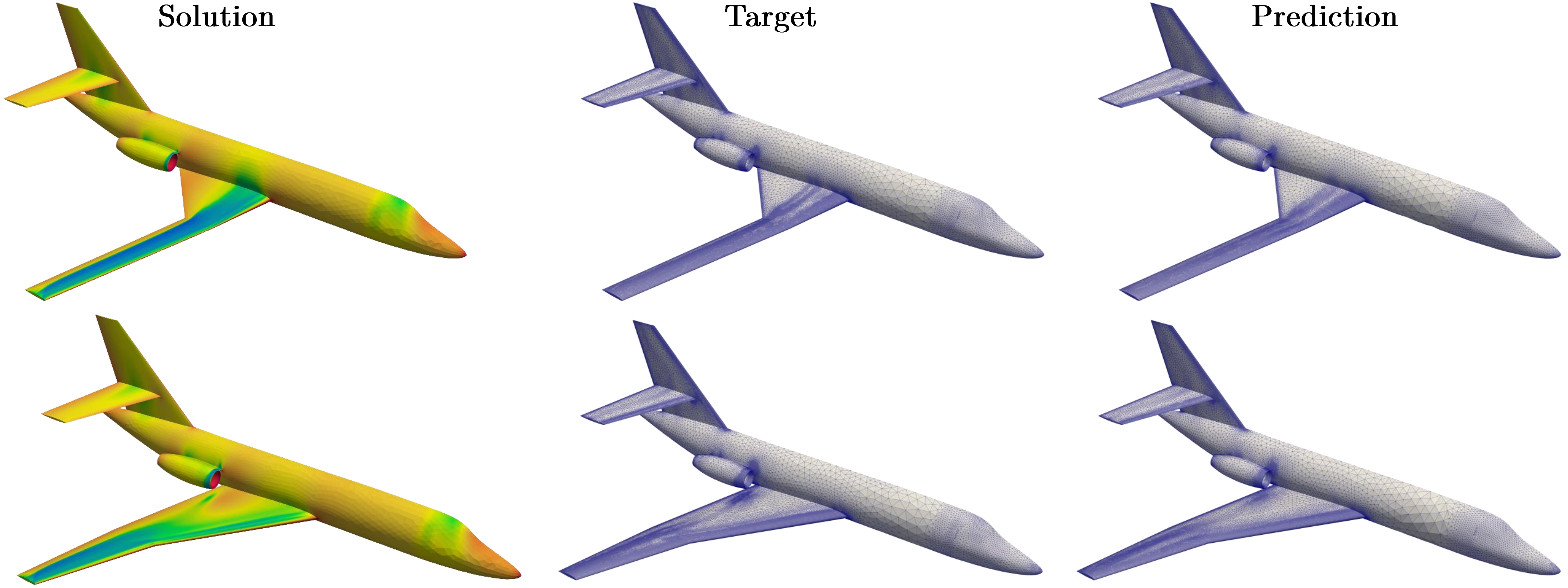
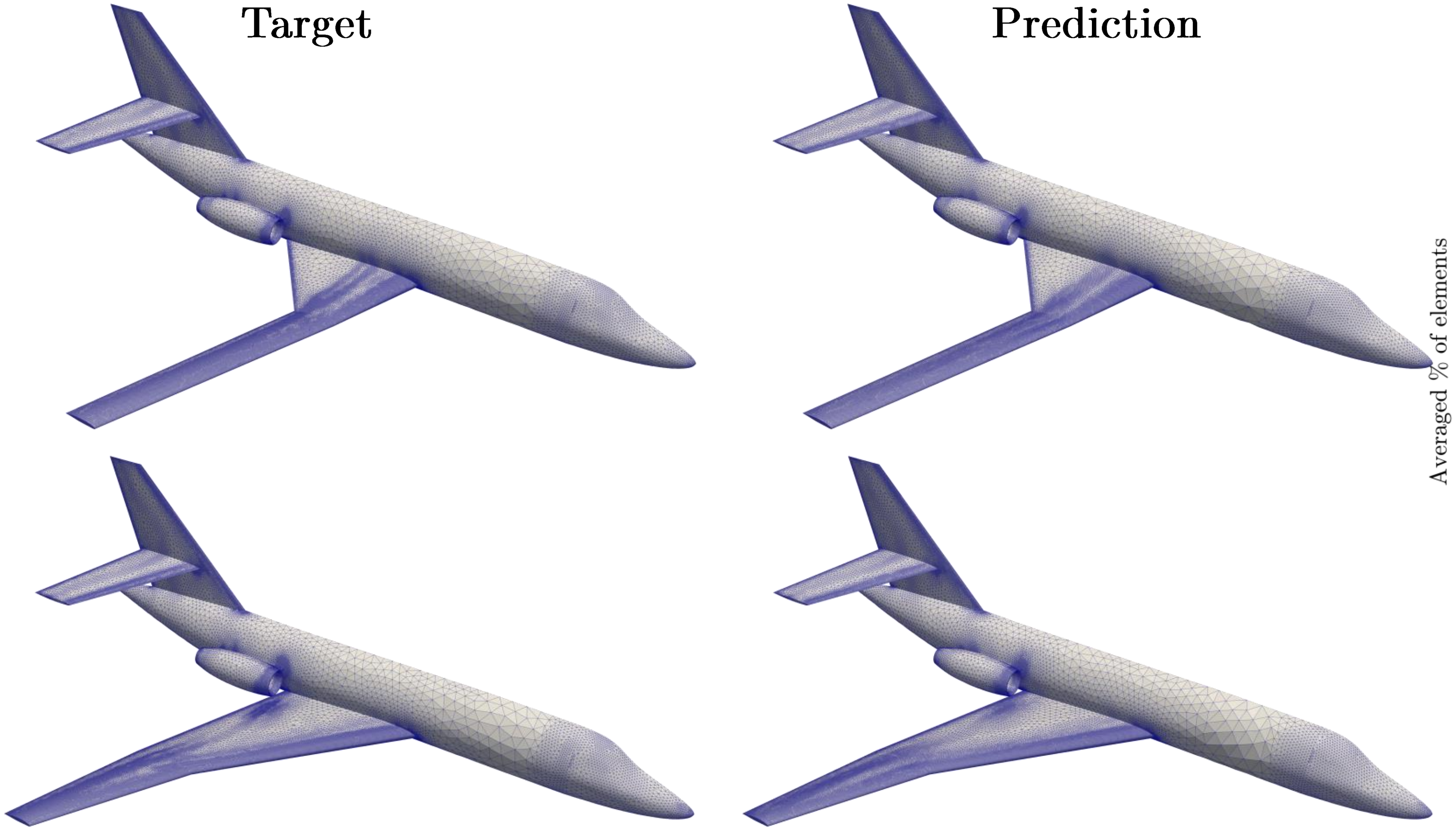
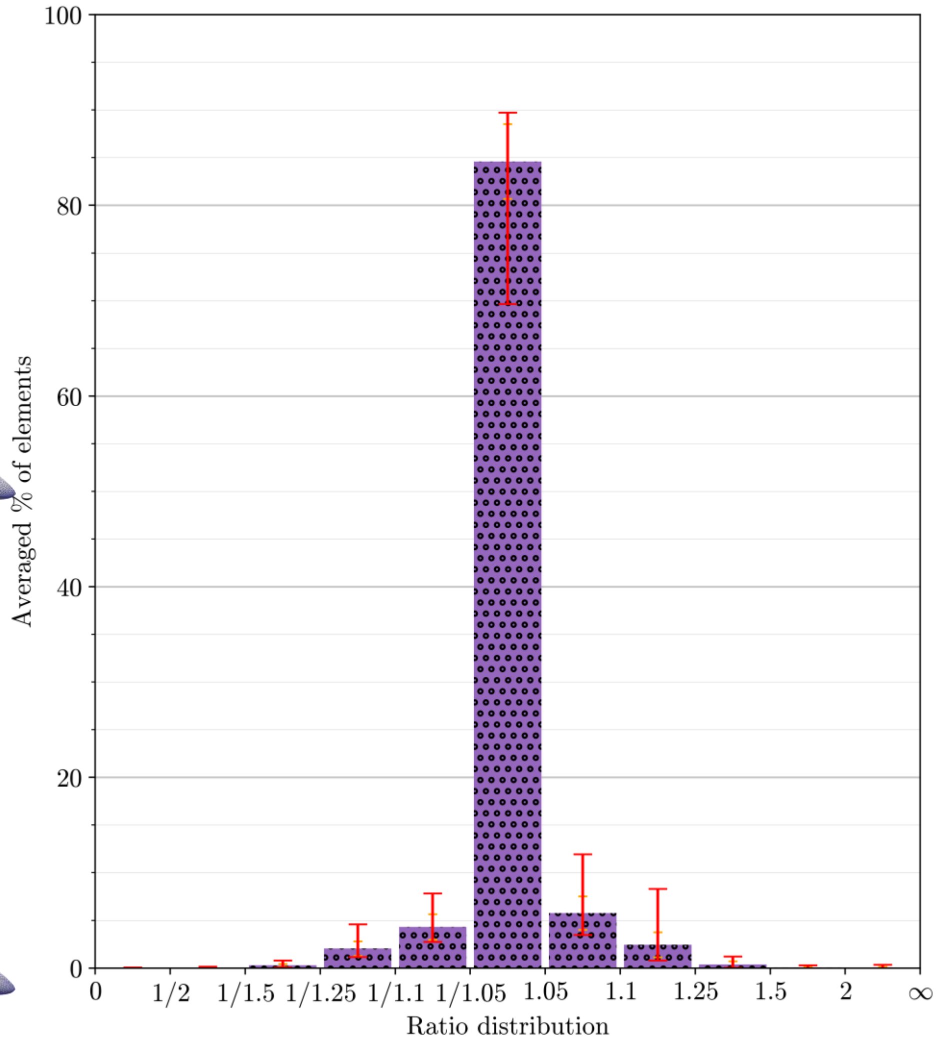


- Spacing at 83% of the points are predicted within 5% of the target

Examples

- Full aircraft – Variable geometry (11 parameters) – 160 training cases
  - Spacing prediction using a background mesh
  - Flow conditions – M=0.8, AoA=2º





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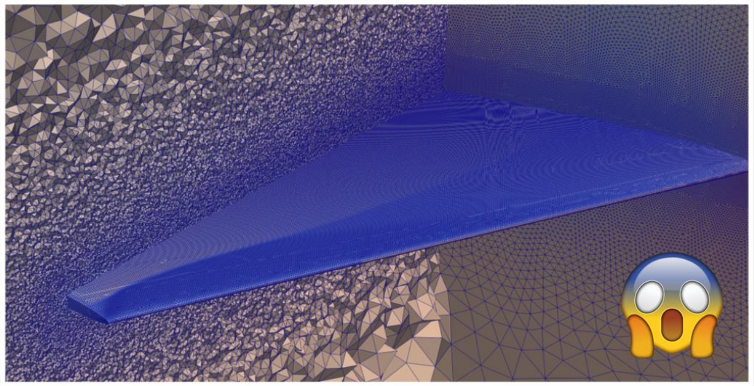
How green is the AI system?

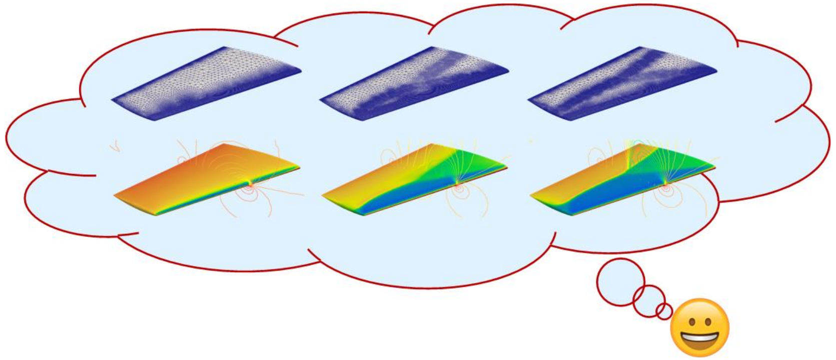
- Carbon footprint for the parametric study using a fixed mesh

Task	Wall clock (H)	Carbon (Kg CO_2e)	Energy (MWh)
Mesh generation	1.0	3.61×10^{-3}	5.89×10^{-5}
CFD solution	3,432.10	527.17	2.28
Total	3,433.0	527.17	2.28



- Carbon footprint for the parametric study using AI predicted meshes

Task	Wall clock (H)	Carbon (Kg CO_2e)	Energy (MWh)
Mesh generation	23.8	0.32	1.40×10^{-3}
CFD solution	143.0	12.36	5.35×10^{-2}
Total	166.8	12.68	0.055



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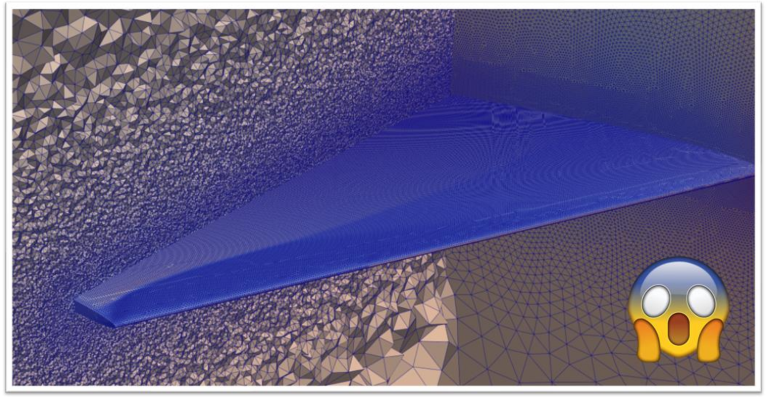
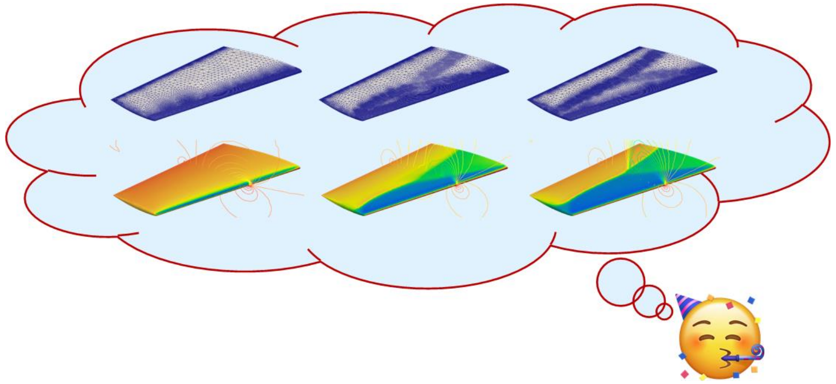


- Carbon footprint for the parametric study using AI predicted meshes

Task	Wall clock (H)	Carbon (Kg CO_2e)	Energy (MWh)
NN tuning and training	156.6	2.13	9.22×10^{-3}
Mesh generation	23.8	0.32	1.40×10^{-3}
CFD solution	143.0	12.36	5.35×10^{-2}
Total	323.4	14.81	0.064



TOTAL carbon footprint is more than 35 times lower

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Concluding remarks

- A green AI system to predict near-optimal mesh spacing for new simulations
  - Operating conditions
  - Geometric variations
- Prediction of mesh spacing within 5% of target for 83% of points for geometric variations involving 11 parameters and using 160 training cases in 3D
- Meshes proved to be suitable to perform simulations of unseen cases

- Current work focuses on
  - Turbulent compressible viscous flows and CAD integration
  - Predicting mesh anisotropy
  - Automatic selection of a background mesh or combine sources and a background mesh

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