

NATIONAL TECHNICAL UNIVERSITY OF ATHENS (NTUA)

SCHOOL OF MECHANICAL ENGINEERING

PARALLEL CFD & OPTIMIZATION UNIT (PCOpt/NTUA)

Adjoint- and ML-based Optimization in Fluid Mechanics/Aerodynamics

(Research Activities of the Parallel CFD & Optimization Unit of the School of Mech. Eng., NTUA)

(Introduction+4 Parts)

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2026, Athens, Greece

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ERCOFTAC SIG34 – “Design-Optimization”



ERCOFTAC

European Research Community On
Flow, Turbulence And Combustion

- **Introductory Courses to Design Optimization** (Munich: 1999-2000-2001-2003), Athens (2004, International Conference), Manchester (2005), Gran Canaria (2006), Trieste (2007), Berlin (2009), Manching (2011), Wolfsburg (2013), Stockholm (2015), Trieste (2017).
- **After 2017, this Course was “merged” with the bi-annual VKI Course on Optimization.**
- **Thoughts to organize the new Introductory Course in 2027, likely in Germany (DLR, Koeln).**

Part 1: Continuous Adjoint for Gradient-Based Optimization

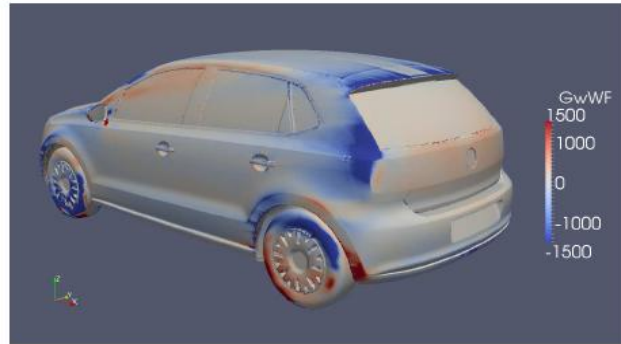
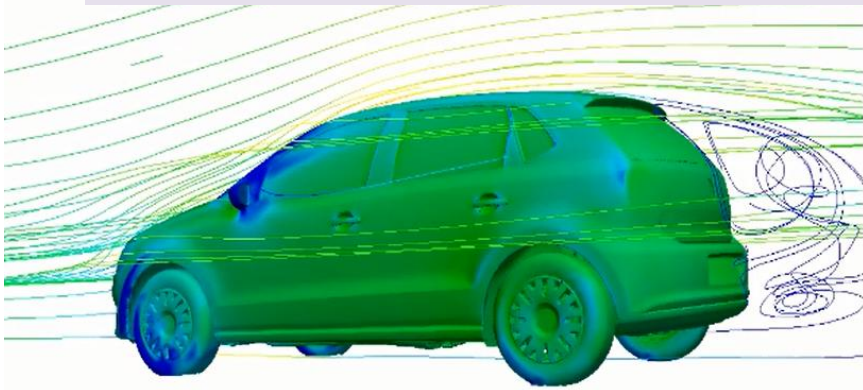
- First-of-its-kind continuous adjoint methods avoiding the “frozen turbulence” assumption. Adjoints to the most widely used turbulence models (Spalart-Allmaras, $k-\epsilon$, $k-\omega$). Adjoint wall functions. Our adjoint solver was made publicly available (*adjointOptimisationFOAM*) through OpenCFD.
- Shape and Topology Optimization (**ShpO**, **TopO**), incl. adjoint for Conjugate Heat Transfer (**CHT**) problems.
- Low cost, adjoint-based computation of higher derivatives for Newton methods and Uncertainty Quantification (**UQ**: Method of Moments, etc.) in CFD.
- The **Think-Discrete-Do-Continuous** (**TDDC**) Adjoint that bridges the gap between discrete and continuous adjoint: use continuous adjoint, with appropriate (“consistent”) discretization schemes and compute gradients as accurate as with discrete adjoint.
- “Similar” adjoint formulations in the GPU-enabled code PUMA (incompressible and compressible flows).

Open  FOAM



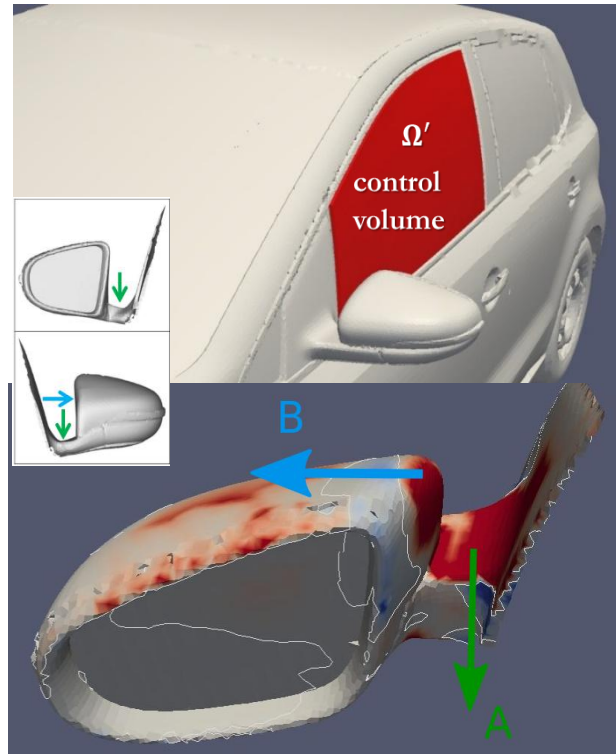
Adjoint-Based Designs for the Automotive Industry – Indicative Applications

- Publicly available adjoint-based ShpO & TopO s/w in the Open ∇ FOAM environment.
- Part of the developed tools (in OpenFOAM) is publicly available (through Open ∇ CFD).

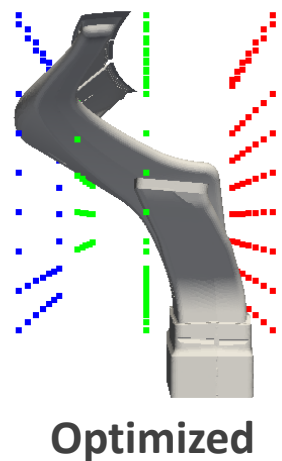
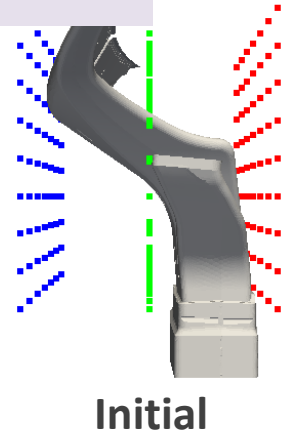


Downforce **sensitivity map** of the VW Polo car. **Red** : move inwards; **blue** : outwards to **increase traction** to the ground.

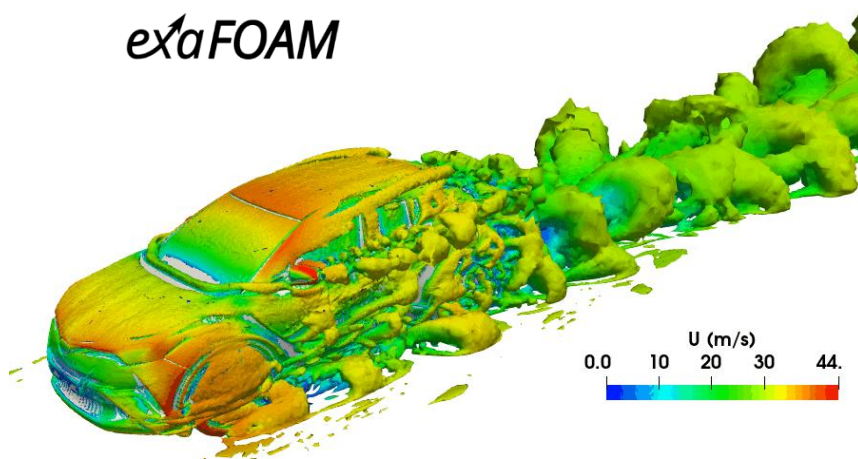
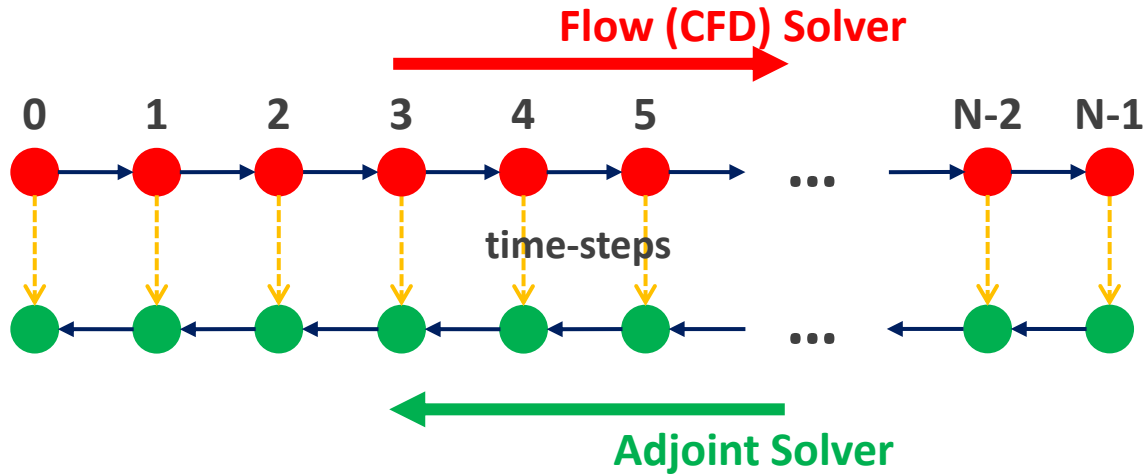
ShpO of the VW Polo **side mirror**, for min. **noise** perceived by the driver.



ShpO of the defroster nozzle of the **HVAC** unit of the YARIS car, for optimal defrosting performance. Manufactured and a defrost test showed that the **windshield defrost time has been reduced by 15%**.

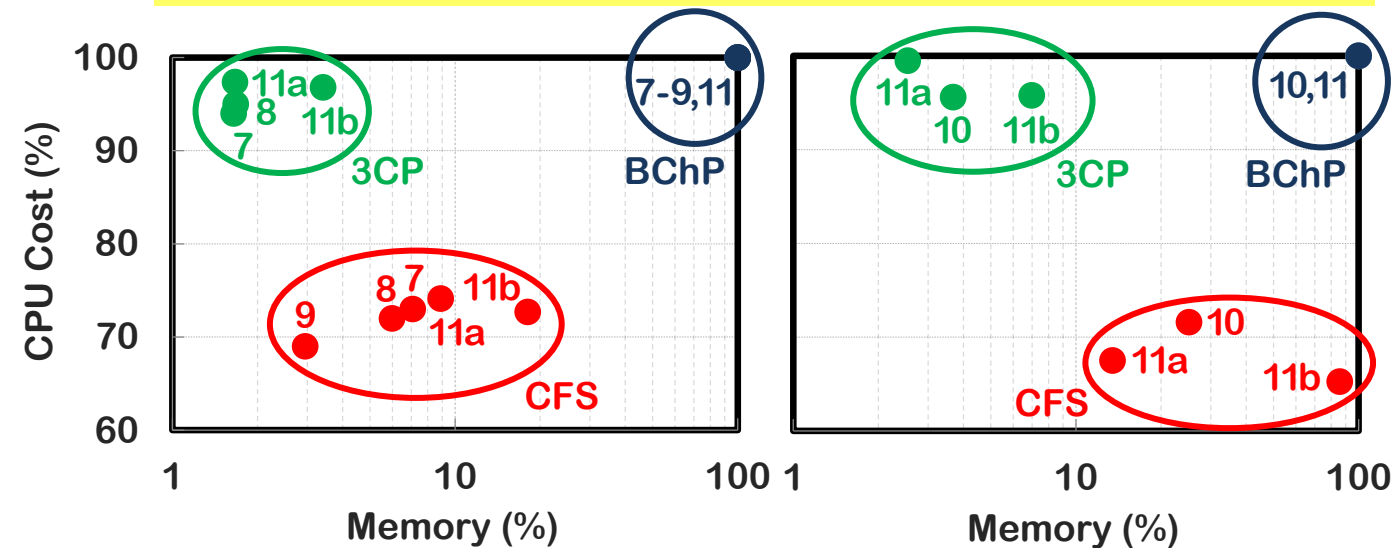


Unsteady Adjoint & Data Compression



Development of compression techniques to keep primal/flow solution time-series in compressed form with/without check-pointing (based on the iPGDZ+ kernel, i.e. a combination of lossy & lossless compression techniques), while integrating adjoint backward in time :

- 4) Compressed Full Storage (**CFS**).
- 5) Compressed Coarse-grained Check-Pointing (**3CP**).

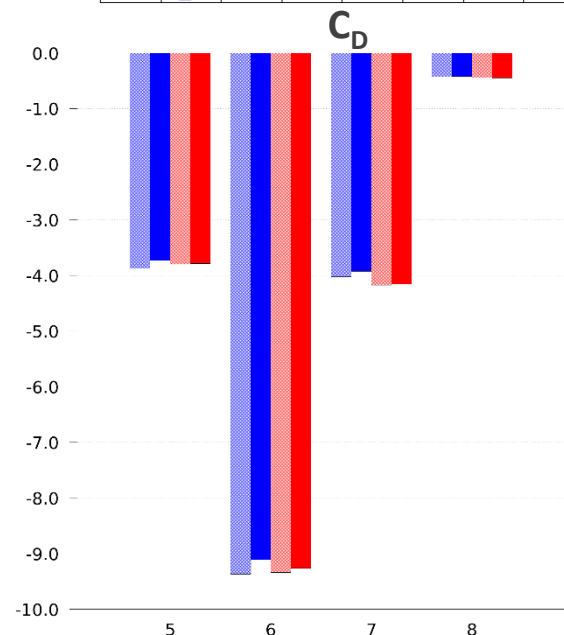
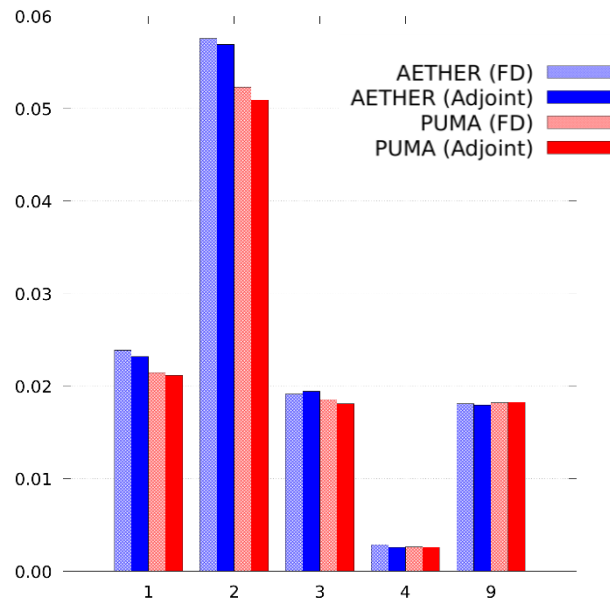
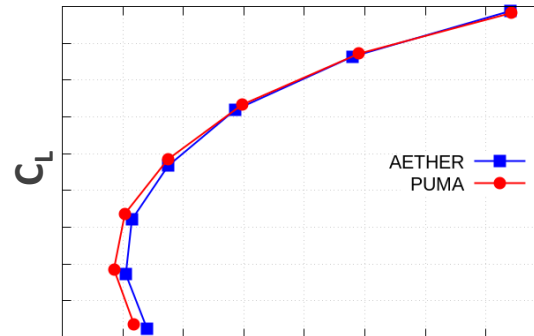
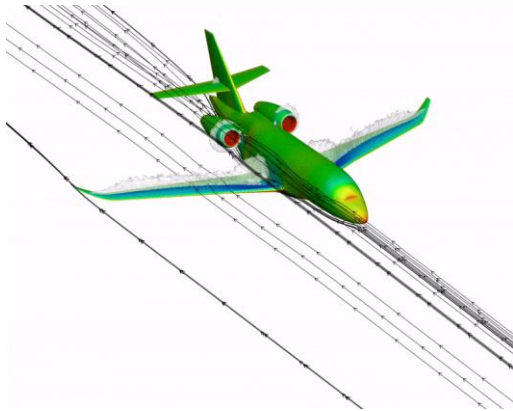


Results from the 5 **URANS** cases

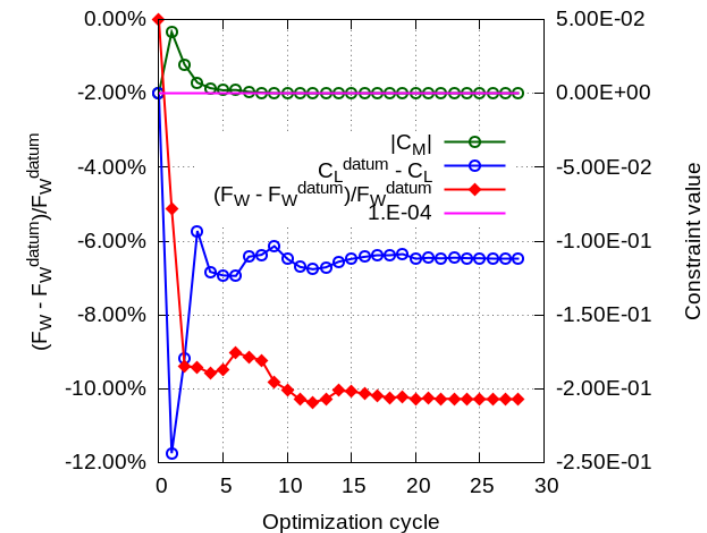
Results from the 3 **DDES** cases

The PUMA s/w: Aero-Structural Analysis & Optimization of a Generic Business Jet

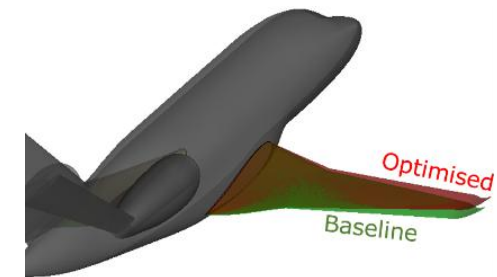
Rigid-wing polar curve (NTUA vs. )



Aero-structural optimization for $M=0.8$, $AoA=2^\circ$. Min. Fuel Burned, subject to constraints on CL and CM .



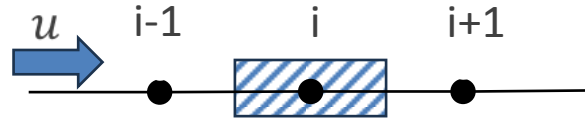
10% reduction in fuel burned, 8% increase in CL/CD , 2% reduction in ZFW



The Think-Discrete Do-Continuous Adjoint (TDDC) – The Concept

A convection term in a 1D ODE:

$$\frac{du^2}{dx}$$



- Upwind 1st order Discretization:

$$\frac{1}{2}(u_i + u_{i+1})u_i - \frac{1}{2}(u_i + u_{i-1})u_{i-1}$$

- Corresponding term in continuous adjoint:

$$2u \frac{d\Psi}{dx}$$

- “Standard”

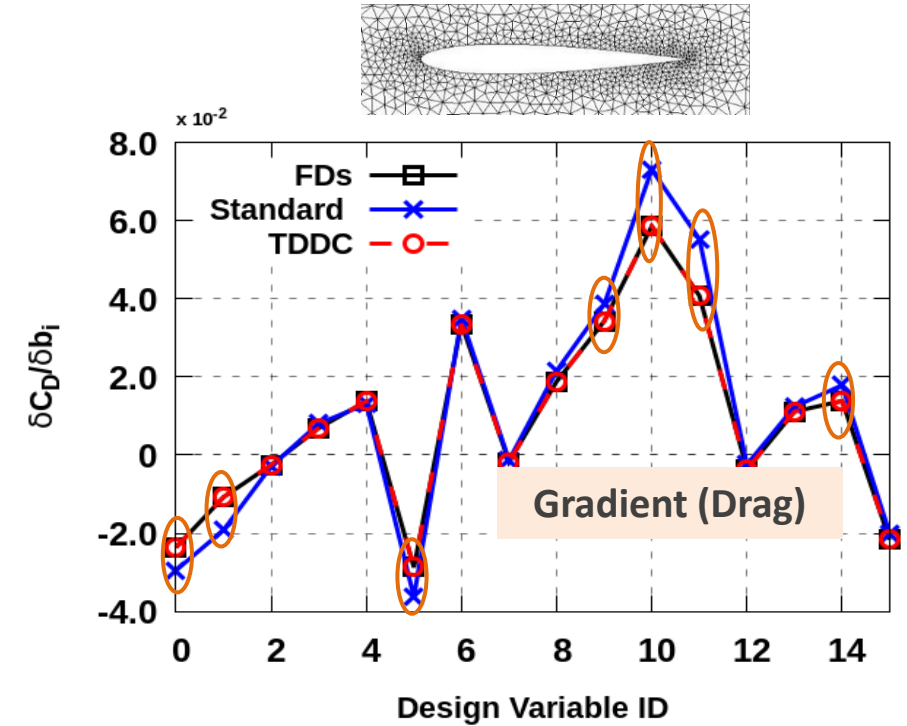
Downwind Discretization:

$$2u_i(\Psi_{i+1} - \Psi_i)$$

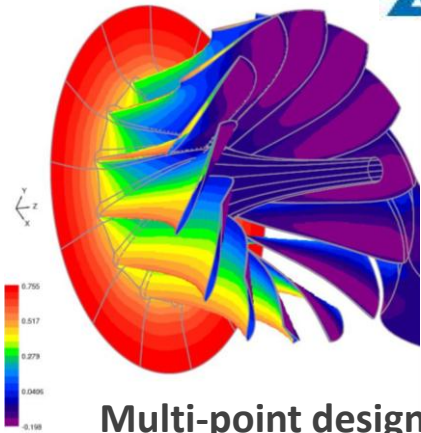
- TDDC Adjoint

“Mixed” Discretization:

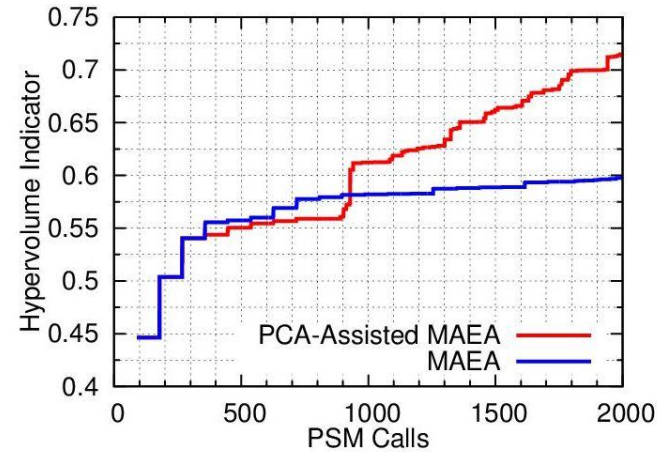
$$2 \left[\underbrace{\frac{1}{4}u_{i-1}(\Psi_i - \Psi_{i-1})}_{\substack{1/4 u \\ \text{upwind}}} + \underbrace{\frac{1}{4}(2u_i + u_{i+1})(\Psi_{i+1} - \Psi_i)}_{\substack{3/4 u \\ \text{downwind}}} \right]$$



Part 2: **EASY** v2.0: Applications in Hydraulic Turbomachines

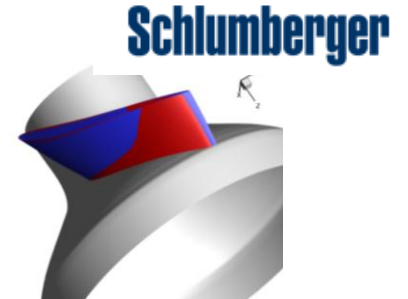
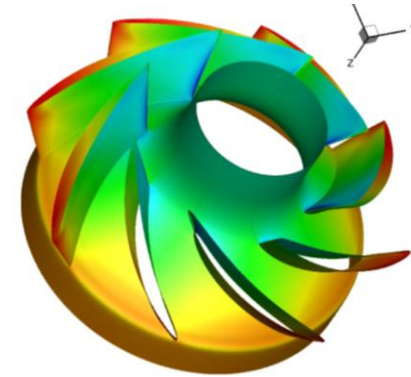


ANDRITZ
Hydro



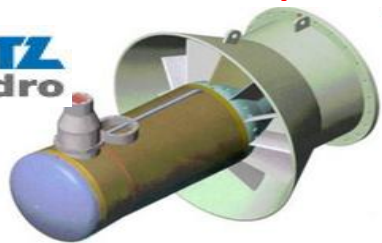
Multi-point design of a Francis runner with **372 design variables**. Due to the extremely high problem dimension, the use PCA-Assisted Metamodels and Evolution Operators in a MAEA is absolutely necessary.

Design of an impeller of a submersible oil drilling pump, with better performance.

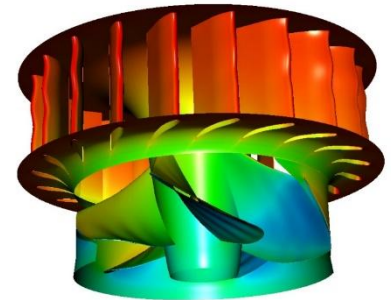


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ANDRITZ
Hydro



In collaboration with Andritz-Hydro, **EASY** was used to design the Hydromatrix®. This is a factory-assembled grid/matrix of small axial-flow, fixed blade type turbine generator units, suitable for low head hydropower sites.

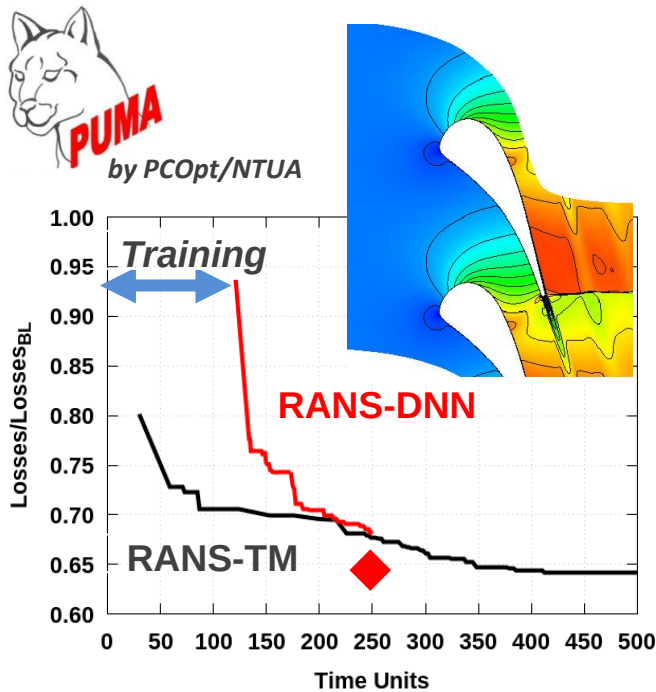


Design of a propeller turbine runner- guide vane stage.

The EASY (Evolutionary Algorithm SYstem) Platform web page <http://velos0.ltt.mech.ntua.gr/EASY>

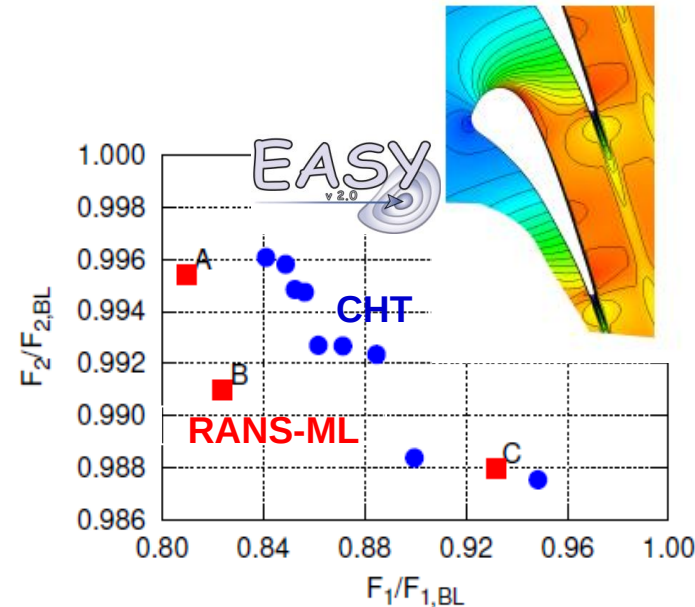
Part3: Some Activities in the field of ML, in the PCOpt/NTUA

Following a >25y research on the use of AI-tools to support evolutionary optimization (the **EASY** platform), when used with costly evaluation tools, during the last 5y research focused on:



(1) ML models as surrogates for Turbulence and Transition models.

Analysis & EA-based optimization of a Highly Loaded Transonic Turbine Blade Cascade. 50% reduction in the optimization cost.

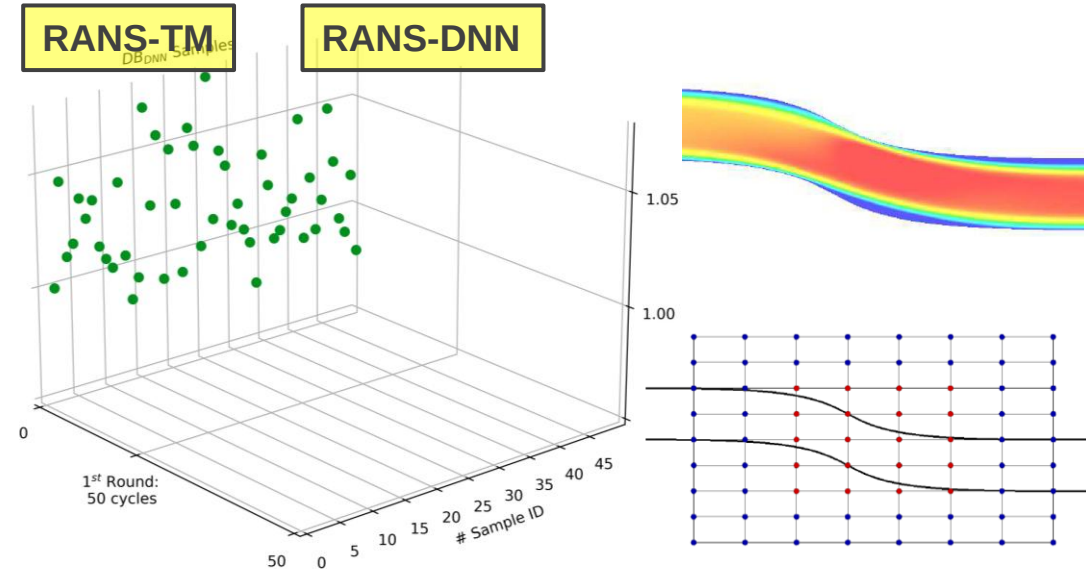


(2) ML models replacing disciplinary solvers in MDO loops.

Aerothermal EA-based optimization of an Internally Cooled Turbine Blade; the **λ -DNN** is used to replace the heat conduction eq. solver over the solid.

Comparison at the same cost.

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(3) Gradient-based ShpO in which differentiated DNNs or PINNs replace the adjoint code.

For the laminar flow through an S-Bend duct, the DNN predicts both F (total pressure losses) and ∇F to be used in gradient-based ShpO, running inexpensively from all training patterns.

CAD into the Optimization Loop - The DLR-F25 transport aircraft

Funded by  
Funded by the European Union



Aerodynamic (Aero-Rigid) & aero-structural (either Aero-Flex or Aero-Structural) ShpO of the high-aspect-ratio wing (HARW) of the **DLR-F25 aircraft** (Small-Medium-Range airliner), with objectives and flight conditions defined by **DLR/AIRBUS**, **without having access to the CAD model**.



Replace the CAD model with an ML surrogate!

Design Variables (CAD Model):

Only the **wing** shape is free to change!

- ☐ The camber at 6 spanwise sections are controlled by 8 variables each.
- ☐ 5 more variables control the twist angles at 5 (out of these 6) sections.

Overall number of Design Variables:

$N=8 \times 6 + 5 = 53$ CAD parameters.

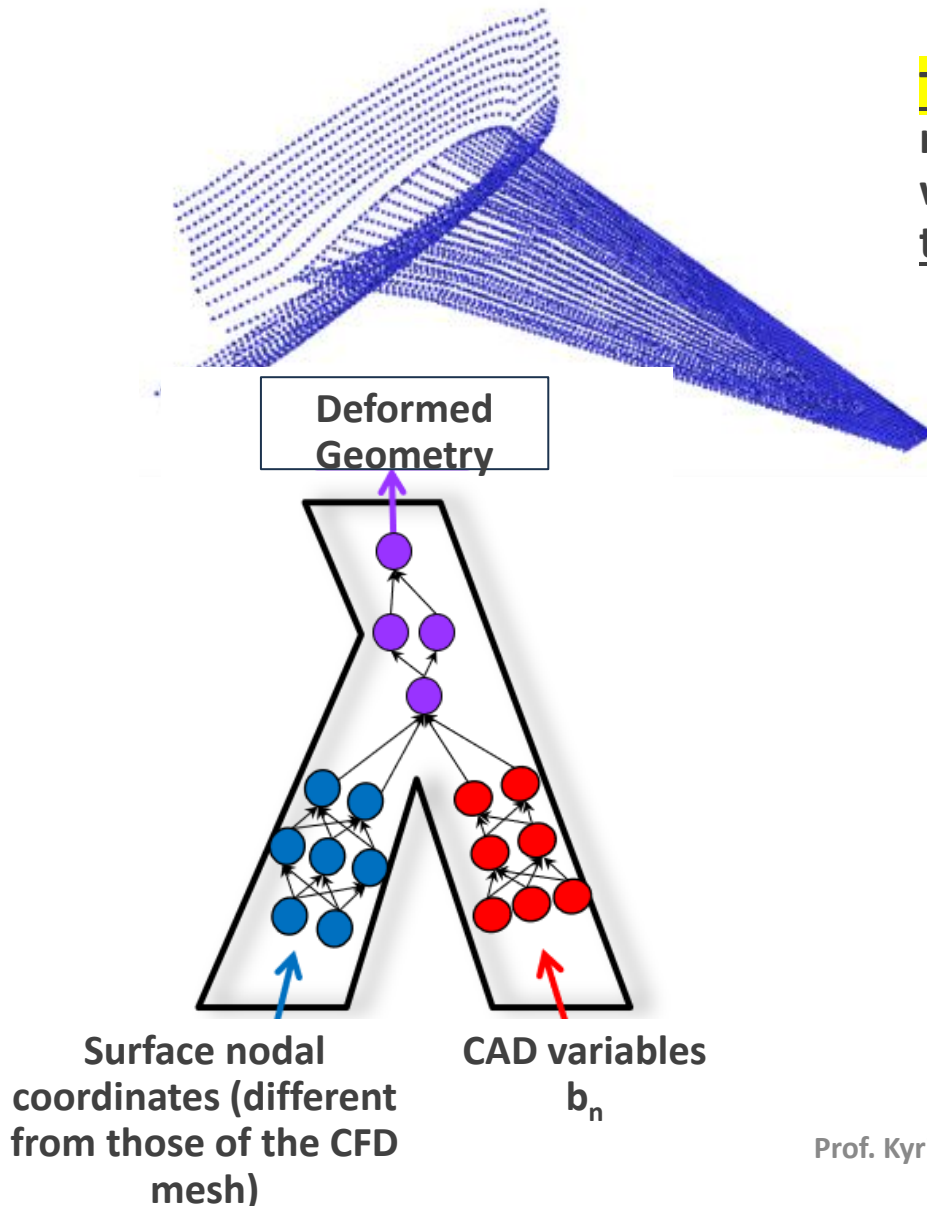
$$\frac{dF}{db_n^{CAD}} = \frac{dF}{dx_i} \cdot \frac{dx_i}{db_n^{CAD}}$$

From the
Adjoint!

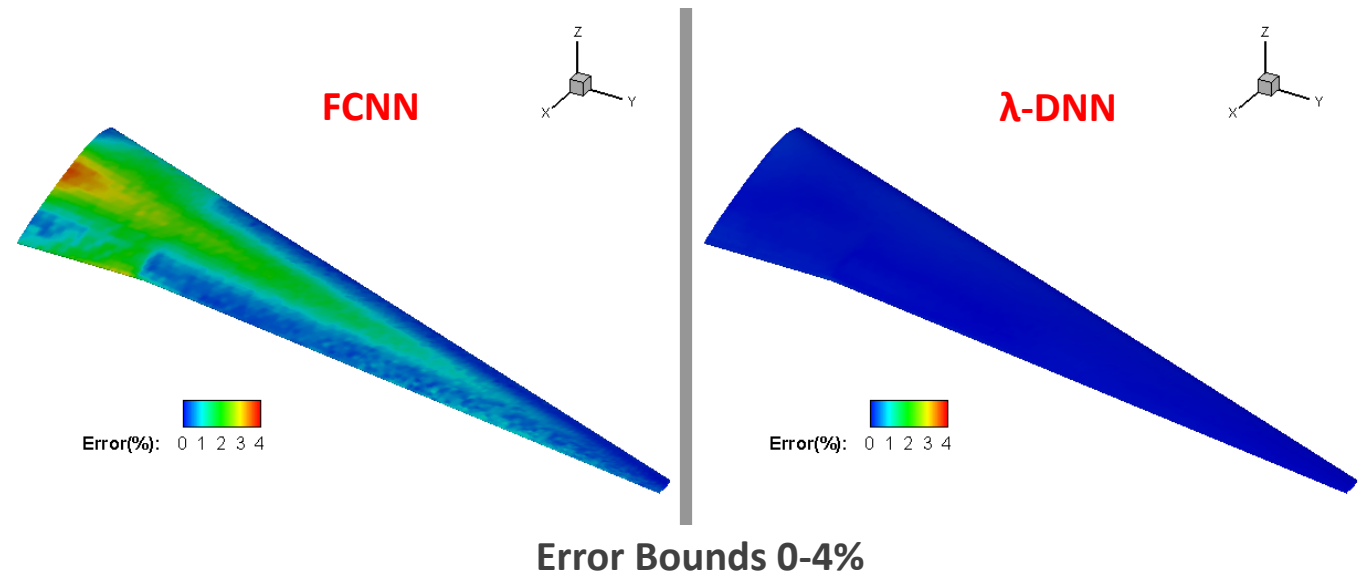
From the
differentiated ML
Surrogate

Training the λ -DNN (a Surrogate for the CAD model)

Training patterns: $K=1992$ aircraft shapes ($N=53$ design variables $\rightarrow P=7080$ nodes), located over the wing and the wing-to-fuselage fairing. 1972 shapes were used for training the λ -DNN, and 20 (plus the baseline; 21 , in total) for testing. An EA (s/w ) optimized the ML hyperparameters.

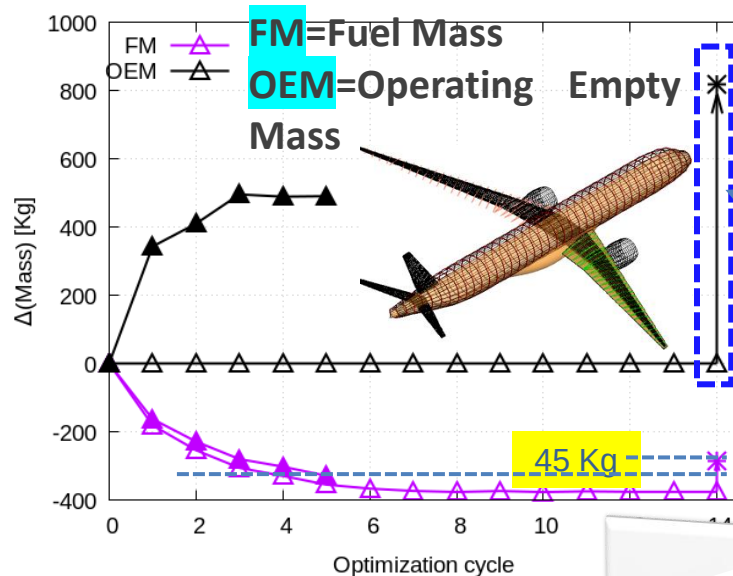
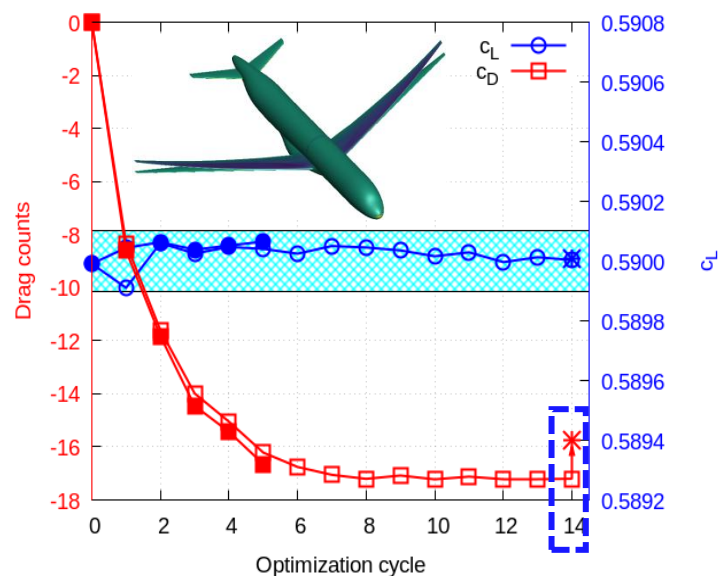


Why the λ -DNN? Prediction Errors on the Wing Surface: FCNN vs. λ -DNN

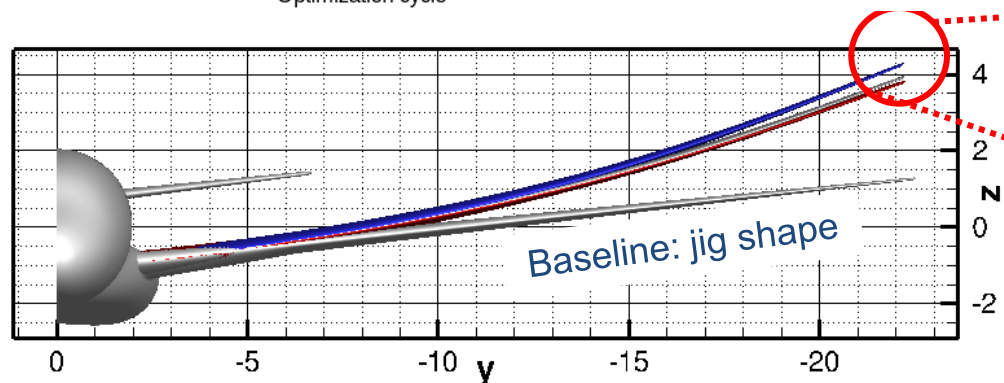


Aero-Structural Optimization

- ✓ Minimize C_D at cruise conditions (same conditions, $C_L=0.59$), fixed HTP = 0° .
- Empty markers: (new) **Aero-Flex** (fixed structural model; aerodynamic objective/constraints) optimization followed by a sizing of the structural model and re-evaluation of aerodynamic performance. Filled marks: **Aero-Structural** optimization.



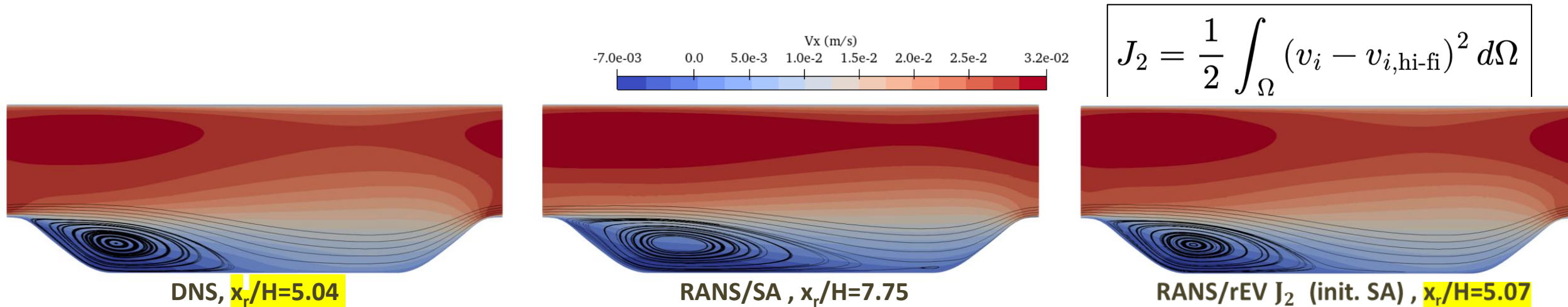
The **Aero-Flex** optimized wing (blue) is highly deflected, calling for a thicker structure to withstand the resulting structural loads. Thickening the wing structure reduces wingtip deflection, bringing the design closer to the aero-structurally optimized one (red).



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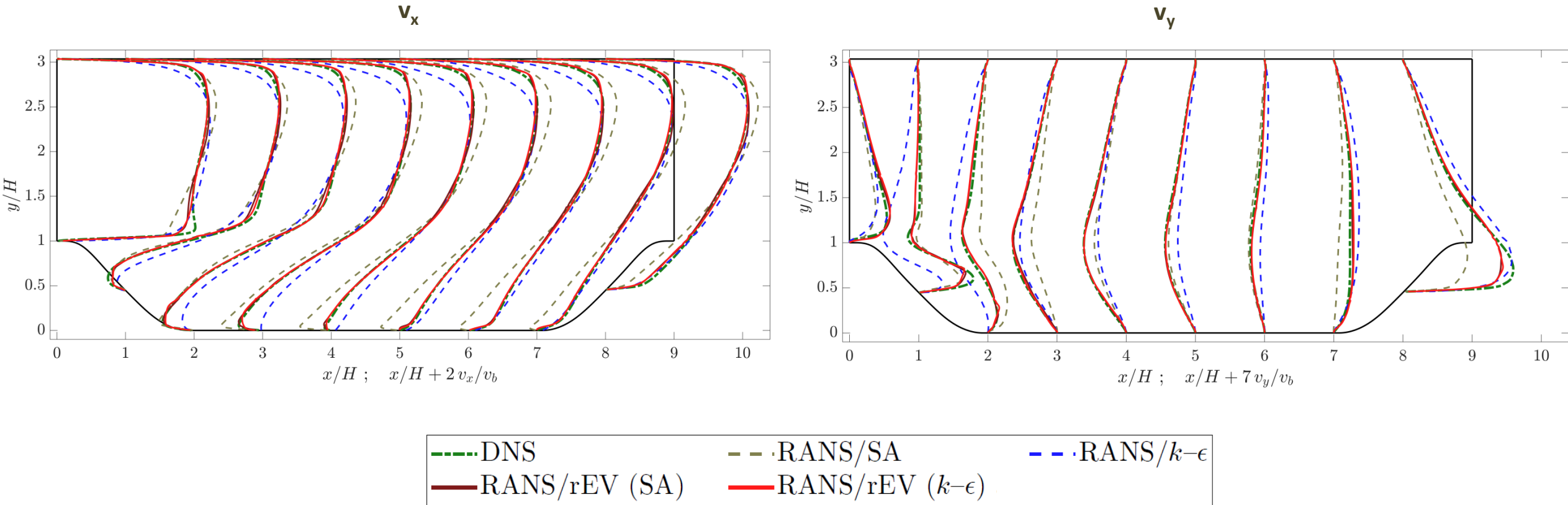
Part4: Low-Cost Gradient-based Optimization with Hi-Fi Models: Field Inversion

- Determine a Correction Field β , to minimize deviations in some fields between hi-fi data and the RANS solver (lo-fi) which the optimization will be based on. The **Eddy-Viscosity Adaptation (EVA, $\beta = \nu_t$)** can be based on either adjoint methods or Physics-informed NN.



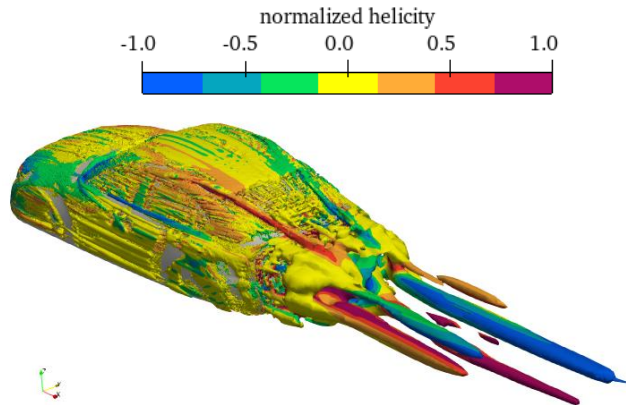
- Perform case evaluations or run ShpO with the updated model. Additionally, use **Symbolic Regression** to build close-form expressions for the EV field, and differentiate them in gradient-based ShpO loops.
- The dual use of adjoint.

Periodic Hills: Computed Velocity profiles

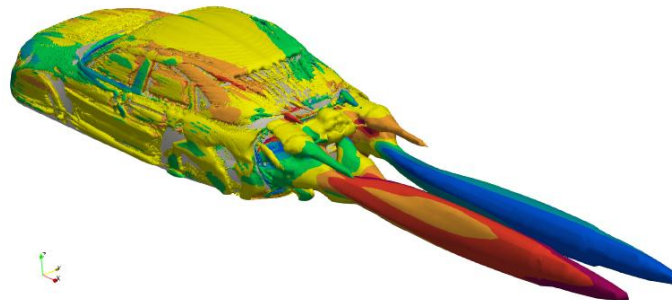


EVA for the DrivAer Fastback (no wheels; no side-mirror) Case

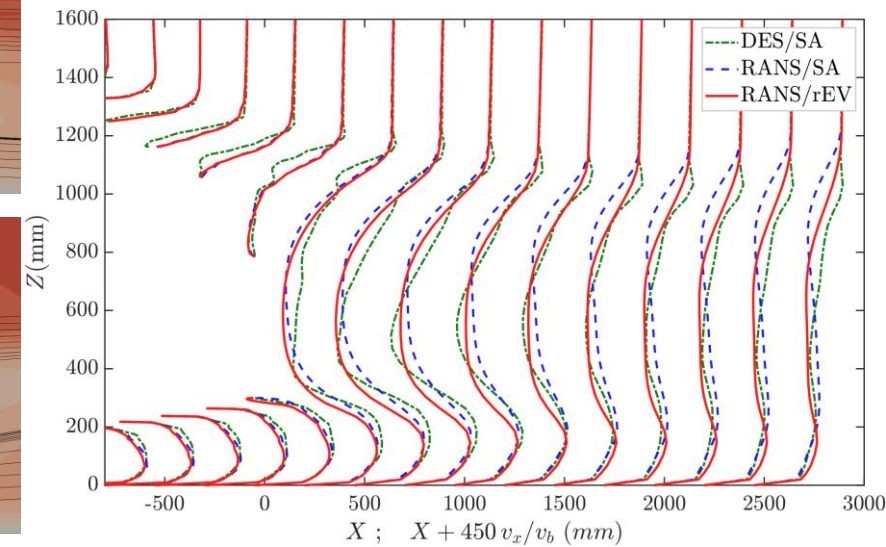
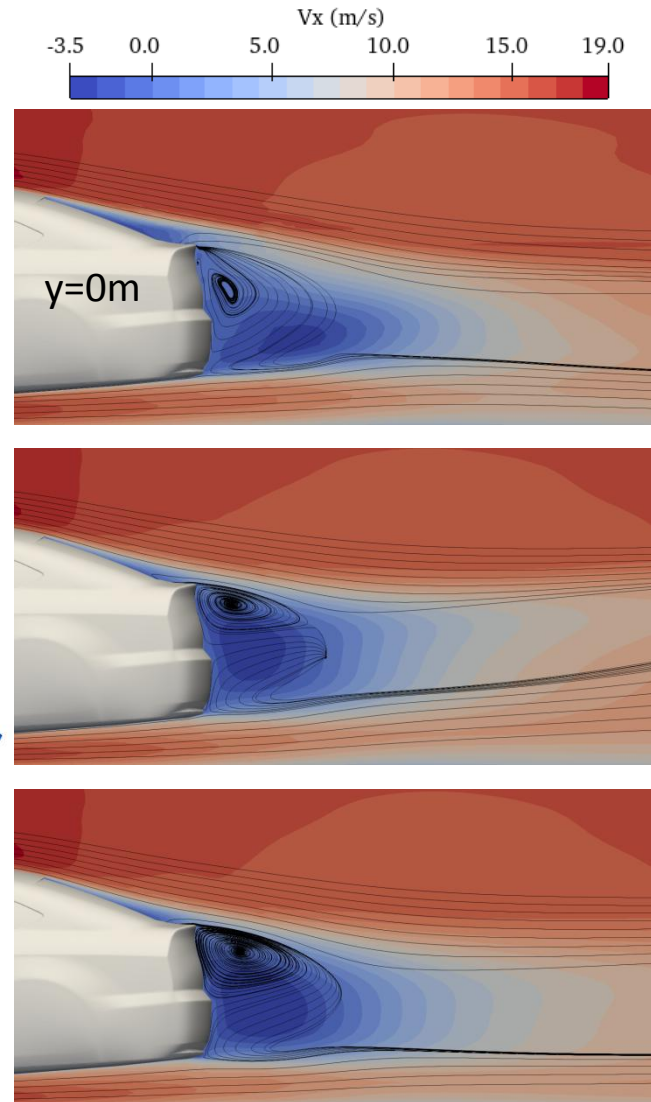
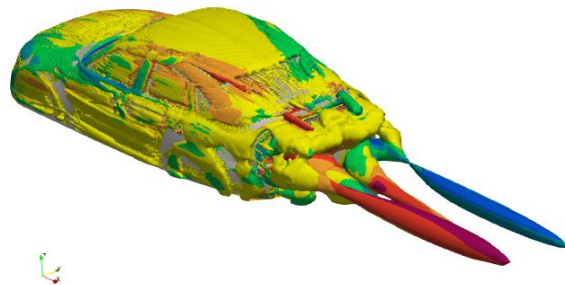
DES/SA, $C_D = 0.113$



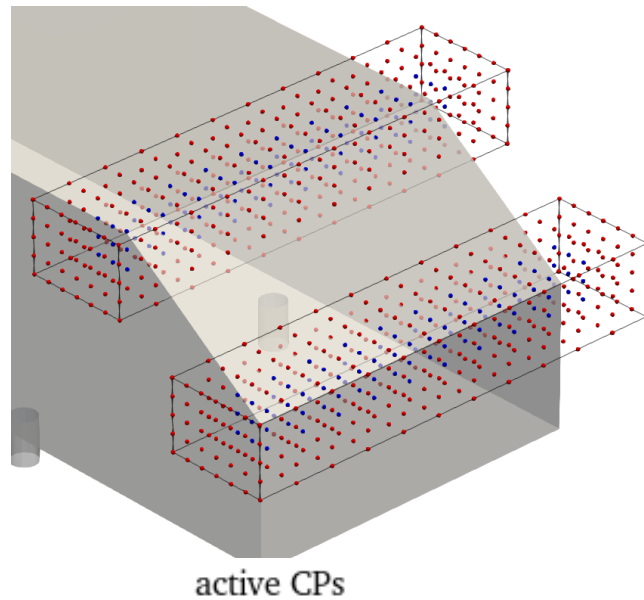
RANS/SA,
 $C_D = 0.132$



RANS/vt[EVA],
 $C_D = 0.124$



ShpO: 35° Slant-Angle Ahmed Body – ShpO using EVA

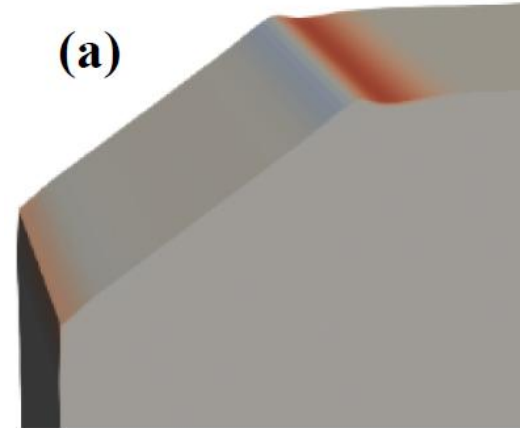


active CPs

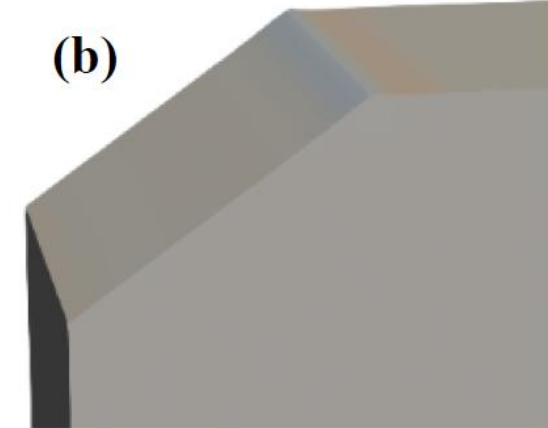
Gradient-based (adjoint) ShpO) options:

rEV → Adjoint running with **raw Eddy Viscosity** (no use of SR)

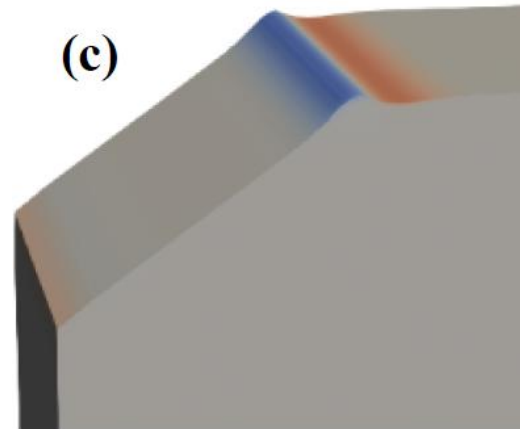
cfEV → Adjoint running with a **closed-form** expression for **Eddy Viscosity** (derived by pySR, a library in Python / **Symbolic Regression**), analytically differentiated whenever needed.



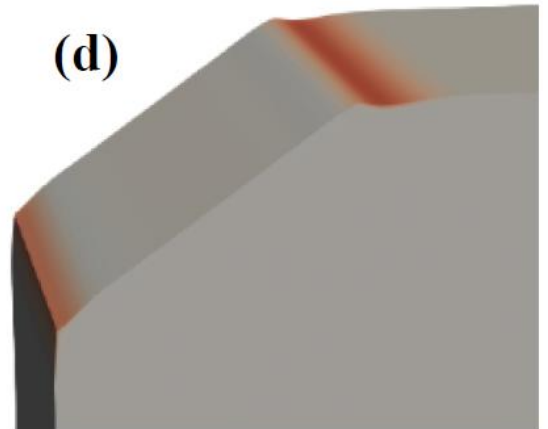
Adjoint to the RANS/SA Eqs.



Adjoint to the RANS, with rEV



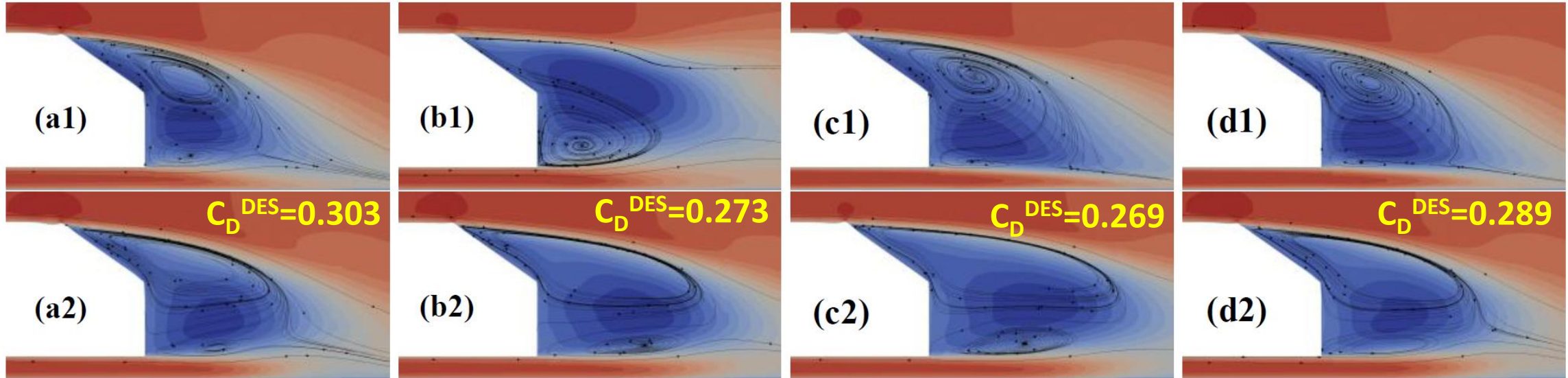
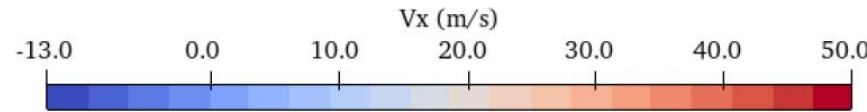
Adjoint to the RANS plus
cfEV (non-differentiated)



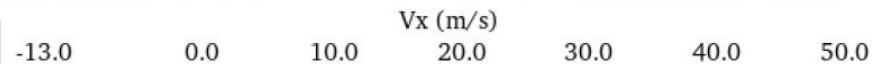
Adjoint to the RANS plus
cfEV (differentiated)

35° Slant-Angle Ahmed Body -4 Optimized Shapes Re-evaluated on the DES-SA Model

Top row: RANS + EVA turbulence model



Bottom row: re-evaluation using DES/SA



Streamwise velocity field and streamlines (black lines) on the symmetry plane, computed by the same model (DES/SA) for the final geometries resulted from the ShpO using the (a) fully differentiated RANS/SA, (b) adjoint to RANS/rEV, (c) adjoint to RANS/cfEV, and (d) the fully differentiated RANS/cfEV.

Original geometry $\rightarrow C_d^{DES} = 0.306$.