Building-block flow model for large-eddy simulation

Adrian Lozano-Duran
MIT AeroAstro

Advanced Modeling & Simulation (AMS) Seminar Series

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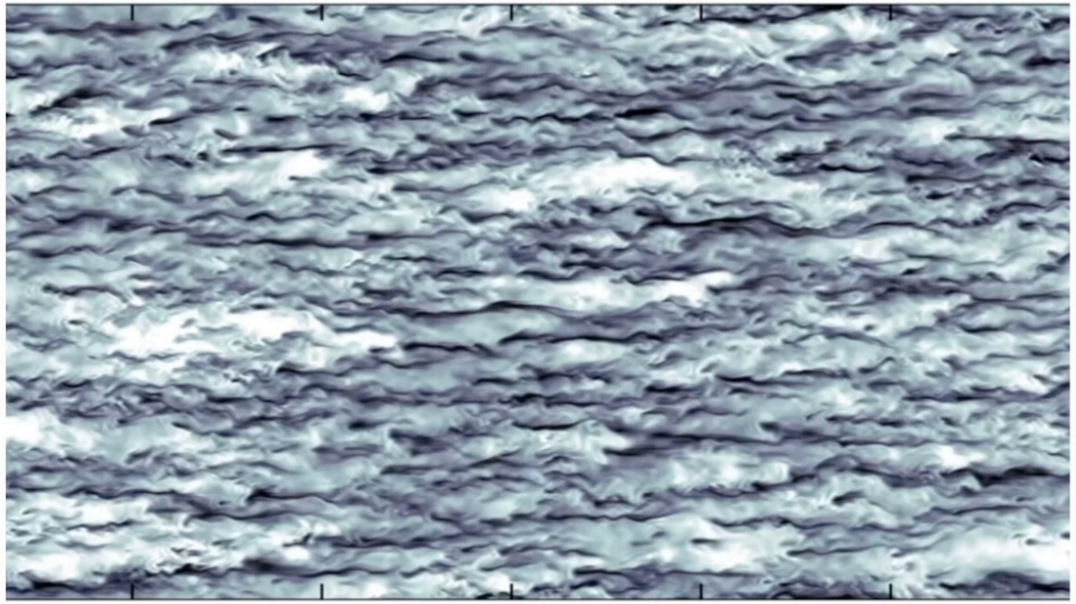
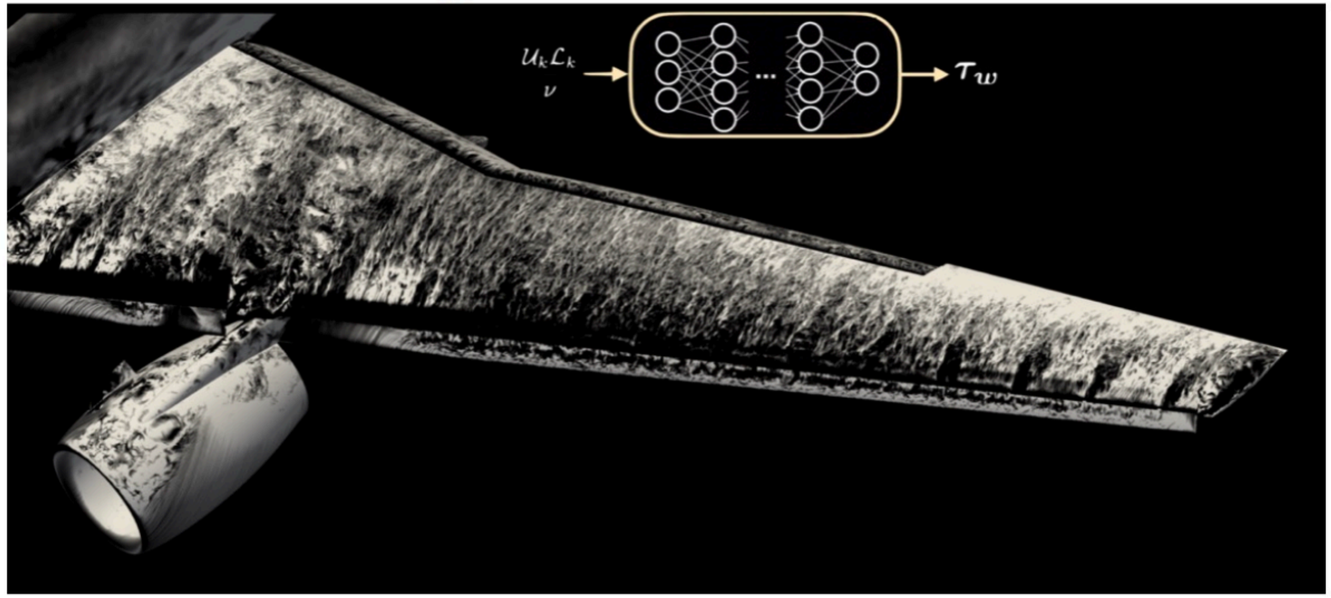
About me

Physics of turbulent flows



- **Physical understanding** of wall-bounded turbulence by devising conceptual models with embedded cause-and-effect relations.
- **Cases**: **separation**, statistical **unsteadiness**, **laminar-to-turbulent transition**, **mean-flow three-dimensionality…**
- **Approach: cause-and-effect** analysis of high-dimensional, chaotic systems.

Turbulence **modeling**



- **Closure models** for turbulence accounting for separation, unsteadiness, mean-flow 3-D, **informed** by the cause-and-effect analysis.
- **Cases:** external aerodynamic applications **(aircraft, rotorcraft,…)**
- **Approach**: large-eddy simulation, machine learning, information theory, HPC,…

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Collaborators

Yuenong Ling

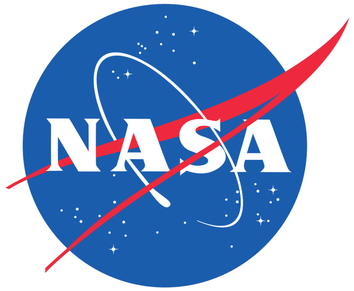
Gonzalo Arranz

Emily Williams

Jane Bae

Konrad Goc

Acknowledgements





Stanford University

Center for Turbulence Research

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Motivation

- Most **qualities** of new aircrafts are currently demonstrated via **flight test**.
- Goal: **Certification by Analysis** Demonstrate aircraft qualities via numerical simulation (Industry & FAA).
- Requirements: **predictions** need to be pushed within the **stringent tolerance** demanded by the industry (<1—3%).



Boeing 787 Dreamliner

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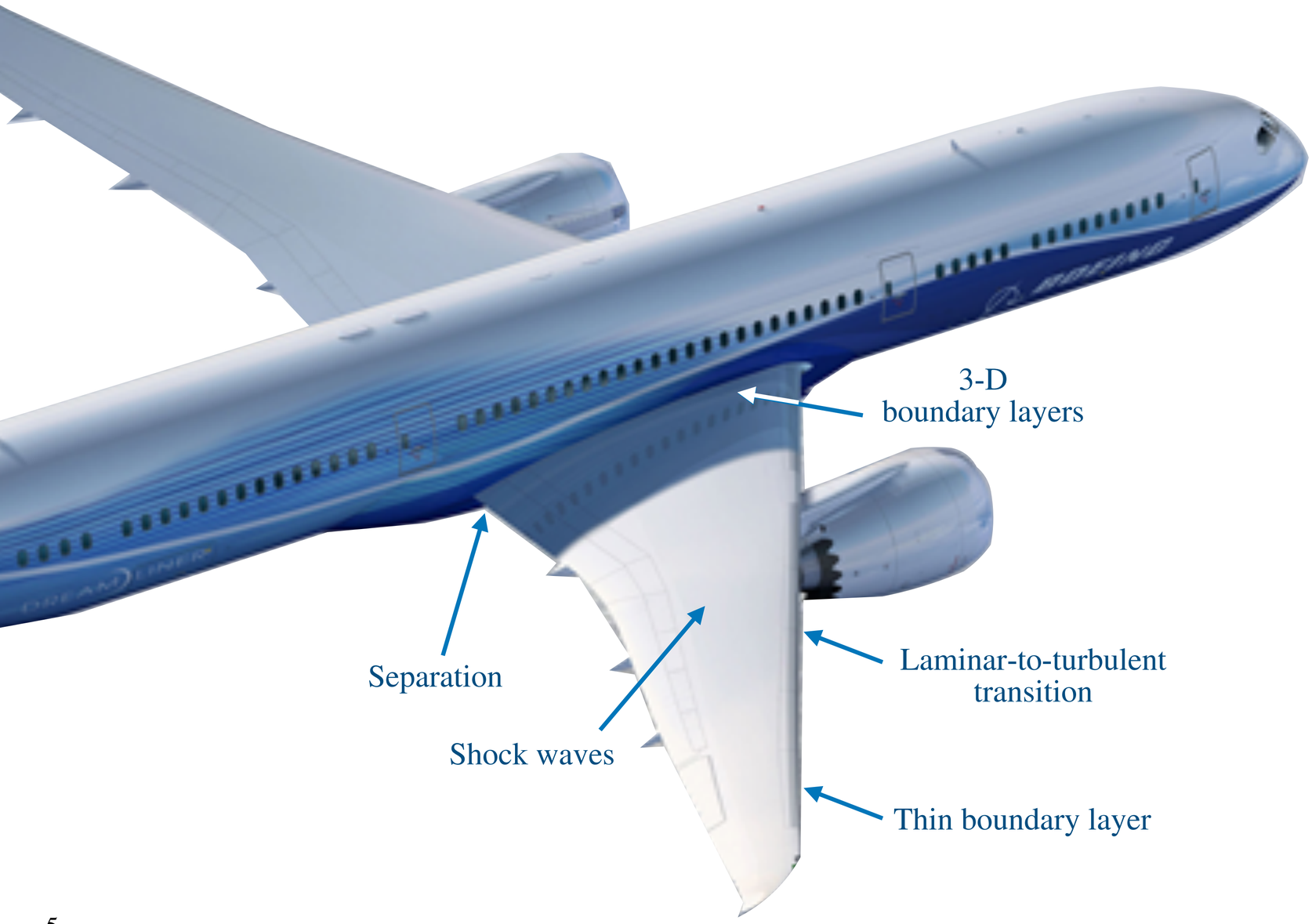
Challenges in numerical simulations of external aerodynamics



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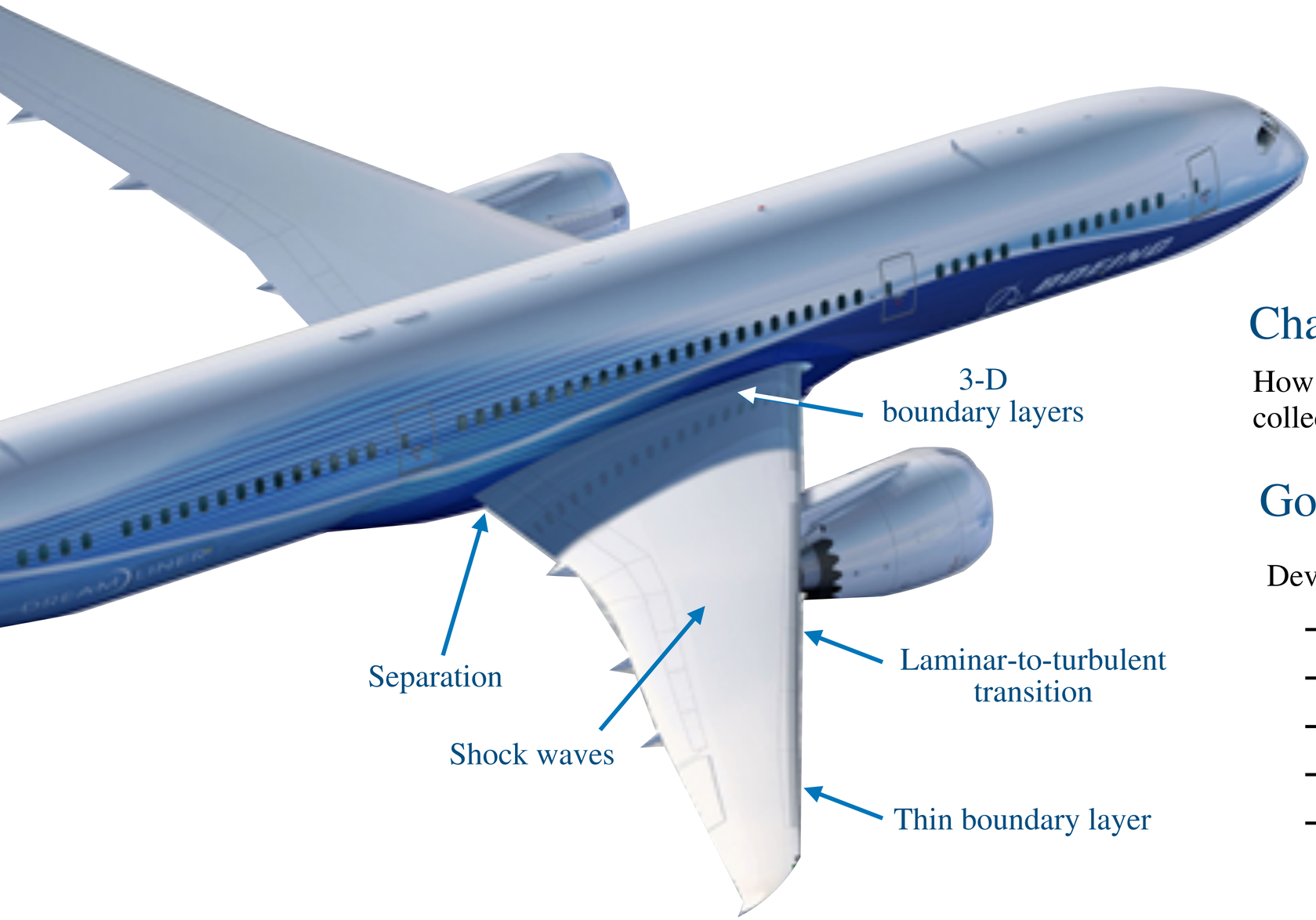
Challenges in numerical simulations of external aerodynamics



Challenge:

How to devise models capable of accounting for rich collection of flow physics in a single unified approach?

Goal:

Devise a model for LES able to

- account for different flow physics
- scalable to additional flows if needed
- consistent with numerical schemes / grids
- provide confidence score in the predictions
- applicable to complex geometries

Outline

Building-block flow wall model:

- Assumptions
- Building blocks
- Model architecture
- Training data

Validation

- Case I: NASA Juncture Flow
- Case II: NASA CRM-HL

Building-block flow SGS/wall model:

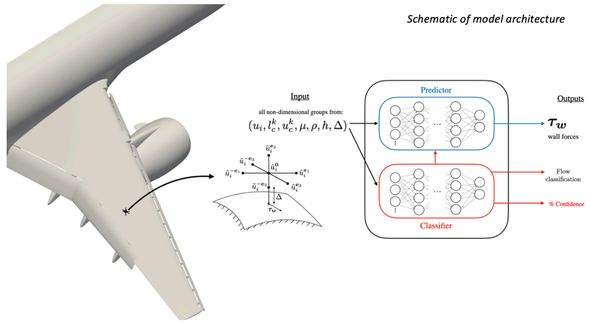
- Validation case: NASA CRM-HL

Limitations

References

Self-critical machine-learning wall-modeled LES for external aerodynamics

By **A. Lozano-Durán AND H. J. Bae†**



Building-block-flow wall-model for large-eddy simulation

Adrián Lozano-Durán*
*Department of Aeronautics and Astronautics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA**

H. Jane Bae
Graduate Aerospace Laboratories, California Institute of Technology, Pasadena, California 91125, USA
(Dated: October 26, 2022)

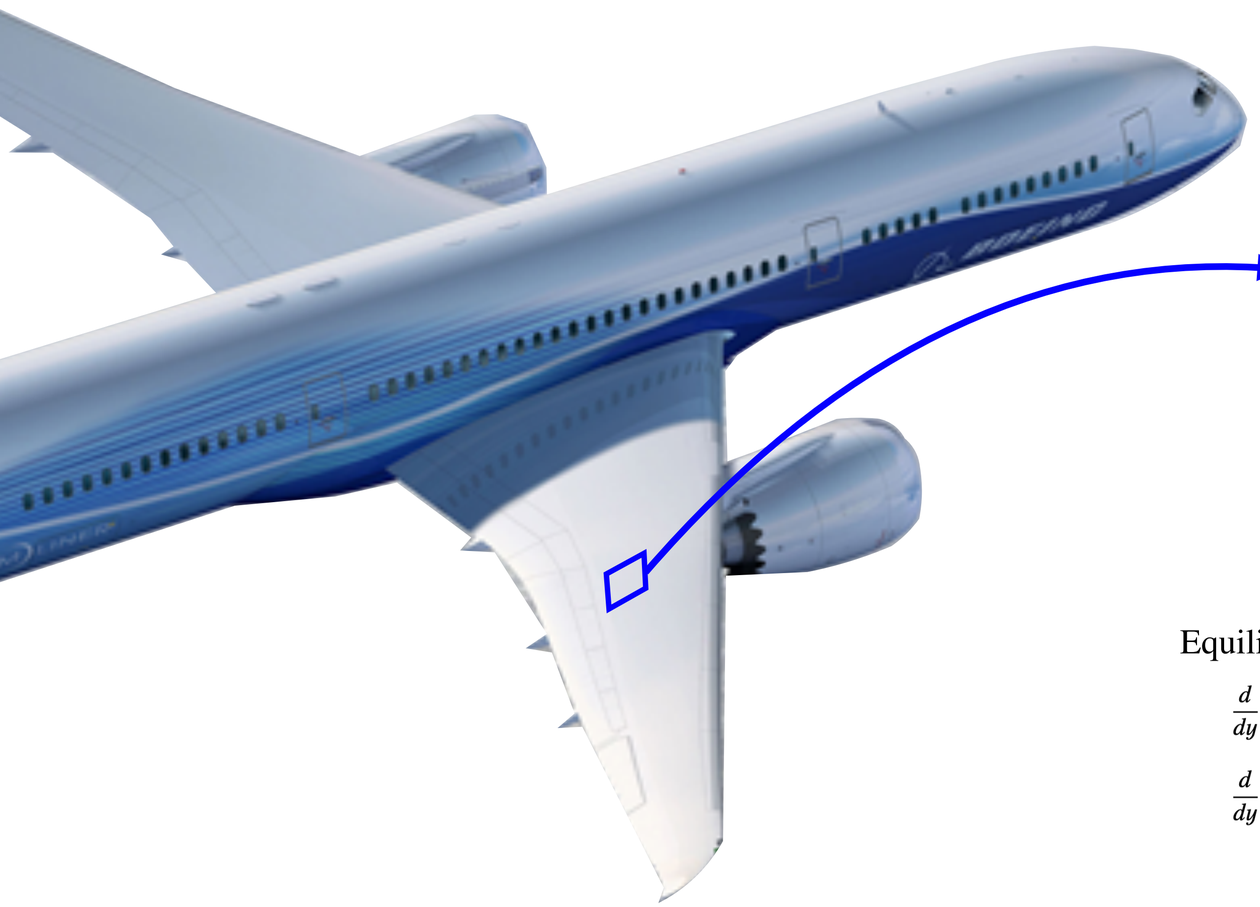
A wall model for large-eddy simulation (LES) is proposed by devising the flow as a collection of building blocks whose information enables the prediction of the wall stress. The core assumption of the model is that simple canonical flows contain the essential physics to provide accurate wall-stress predictions in more complex flows. The model is constructed to predict wall-attached turbulence, favorable/adverse pressure gradient turbulence, separation, statistically unsteady turbulence, and laminar flow. The approach is implemented using two interconnected artificial neural networks: a classifier, which identifies the contribution of each building block in the flow; and a predictor, which estimates the wall stress via non-linear combination of the building-block units. The training data are directly obtained from wall-modeled LES with exact modeling for mean quantities to guarantee consistency with the numerical discretization. The output of the model is accompanied by the confidence in the prediction. The latter aids the detection of areas where the model underperforms, such as flow regions that are not representative of the building blocks used to train the model. The model is validated in two realistic aircraft configurations: High-lift Common Research Model and NASA Juncture Flow Experiment.

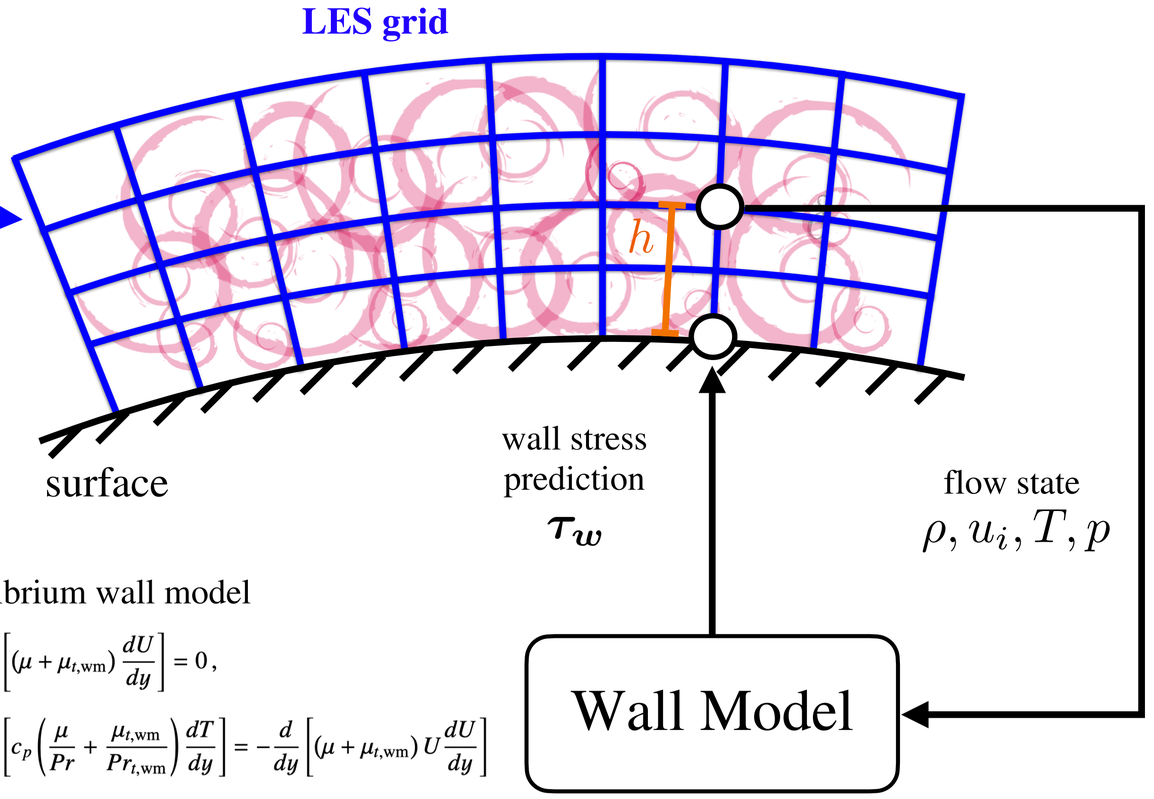
Wall-modeled LES based on building-block flows

By Y. Ling†, G. Arranz†, E. Williams†, K. Goc, K. Griffin AND A. Lozano-Duran†

A unified subgrid-scale (SGS) and wall model for large-eddy simulation (LES) is proposed by devising the flow as a collection of building blocks that enables the prediction of the eddy viscosity. The core assumption of the model is that simple canonical flows contain the essential physics to provide accurate predictions in more complex flows. The model is constructed to predict zero-pressure-gradient wall-bounded turbulence, adverse pressure gradient effects, separation, and laminar flow. The approach is implemented using a Bayesian classifier, which identifies the contribution of each building block in the flow, and a neural-network-based predictor, which estimates the eddy viscosity based on the building-block units. The training data are directly obtained from wall-modeled LES with an exact SGS/wall model for the mean quantities to guarantee consistency with the numerical discretization. The model is validated in the NASA Common Research Model High-lift and shown to improve the predictions with respect to current modeling approaches.

Wall-modeled large-eddy simulation



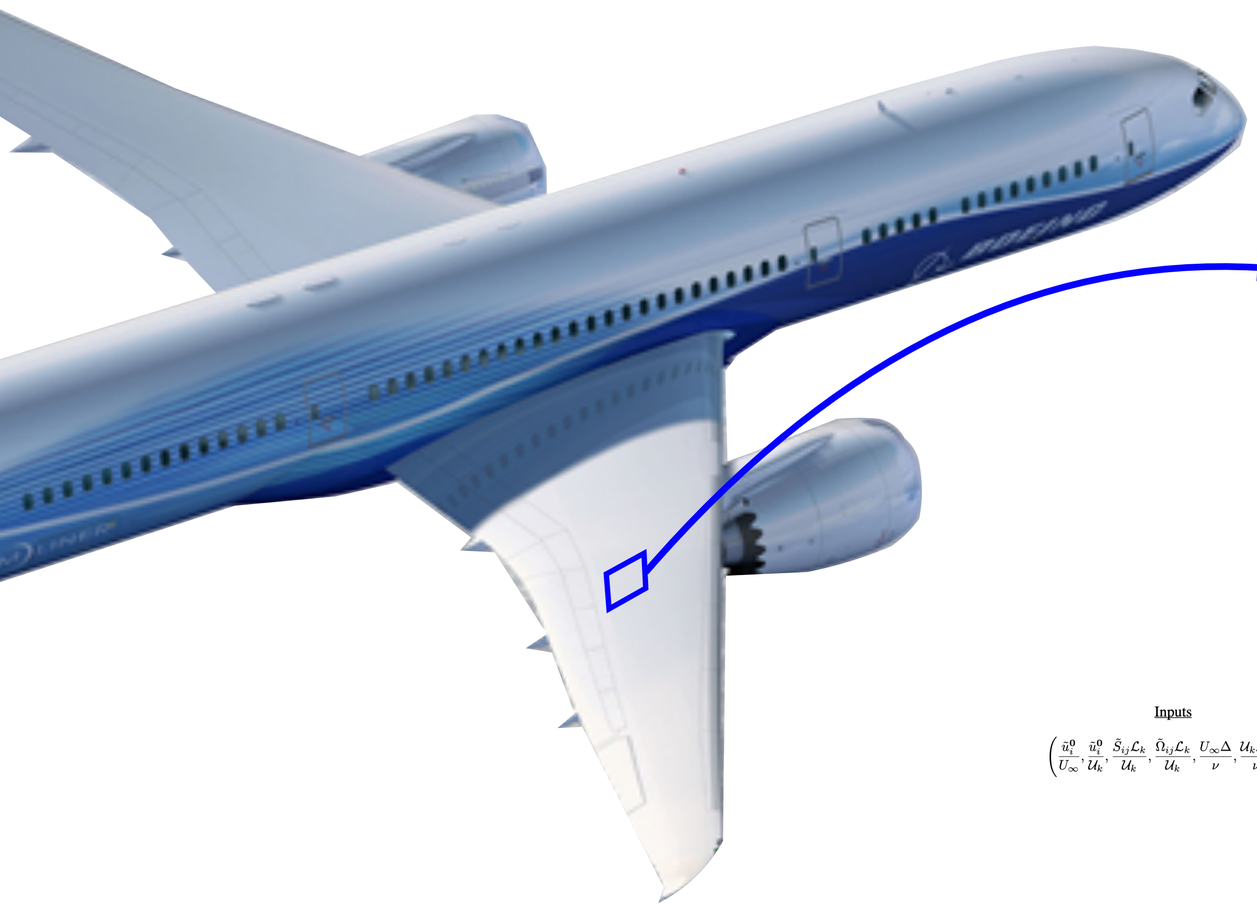


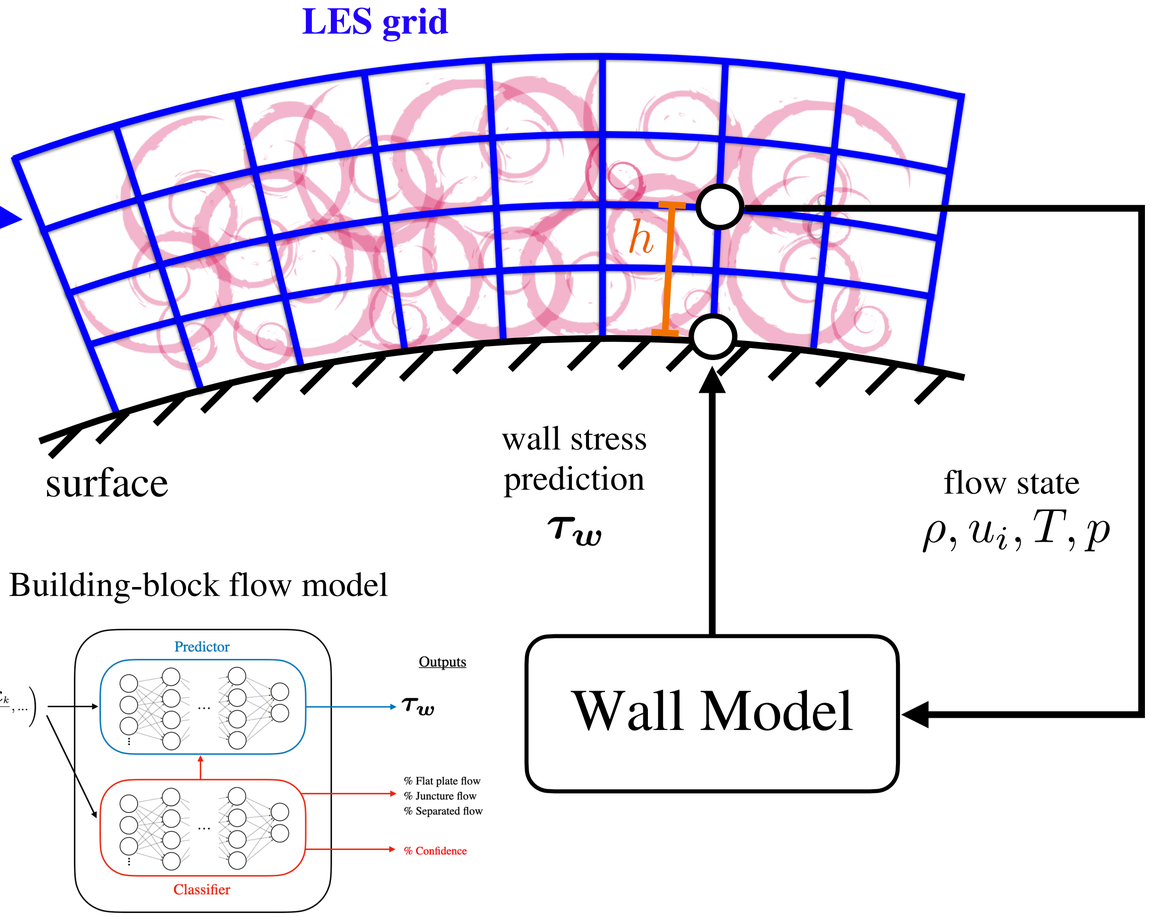
Equilibrium wall model

$$\frac{d}{dy}\left[(\mu+\mu_{t,\mathrm{wm}})\frac{dU}{dy}\right]=0\,,$$

$$\frac{d}{dy}\left[c_p\left(\frac{\mu}{Pr}+\frac{\mu_{t,\mathrm{wm}}}{Pr_{t,\mathrm{wm}}}\right)\frac{dT}{dy}\right]=-\frac{d}{dy}\left[(\mu+\mu_{t,\mathrm{wm}})\,U\frac{dU}{dy}\right]$$

Wall-modeled large-eddy simulation





Building-block flow model:
Assumptions, building blocks, architecture & training data

Building-block-flow model: assumptions

Main model assumptions:

1. There is a finite set of simple flows (referred to as building-block flows) that contains the essential flow physics to formulate generalizable wall models.

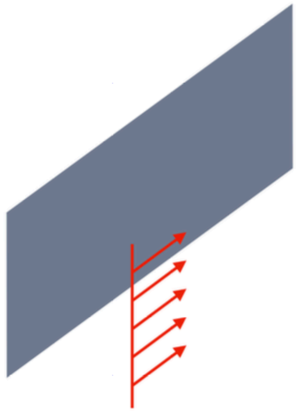
2. The effect of the (missing) near-wall subgrid scales in WMLES are representable by a linear combination of the near-wall behavior of the building-block flows.

3. Flow information from two wall-normal locations is enough to predict the local wall stress in the vicinity of those points.

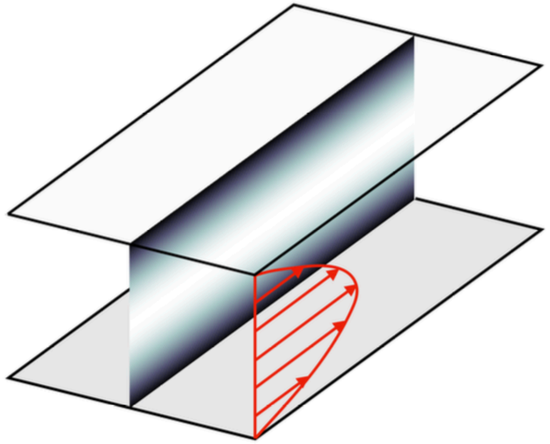
4. History effects for the subgrid-scale flow are captured using instantaneous accelerations without the need of additional information from past times.

Building-block-flow model: building blocks

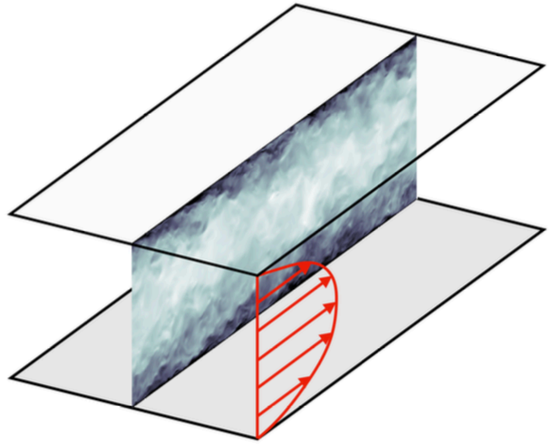
Freestream

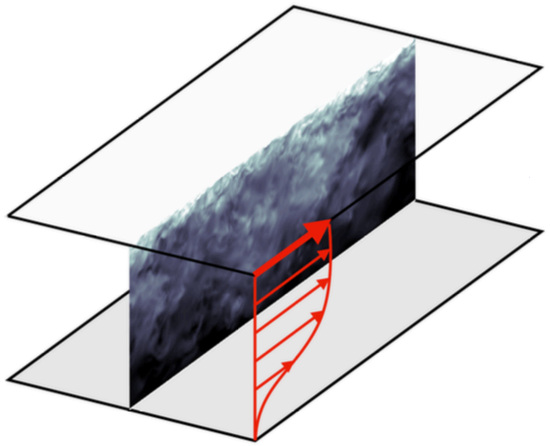


Laminar channel

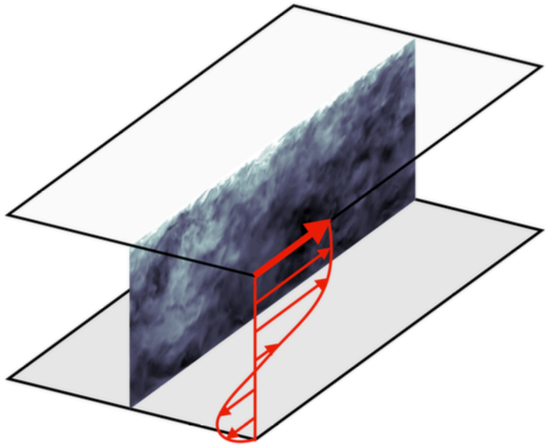


Zero mean-pressure-gradient turbulence (ZPG)
(turbulent channel)

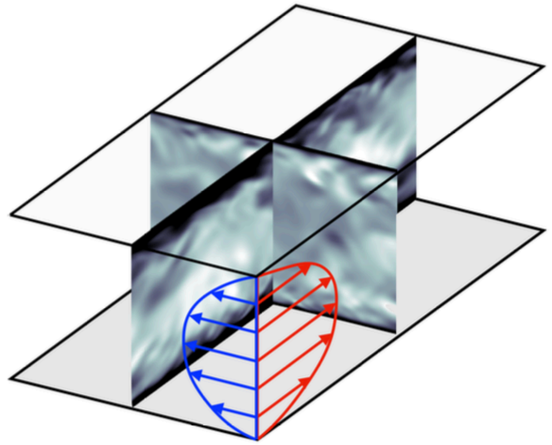




"Separation"
(Turbulent Poiseuille-Couette flow)



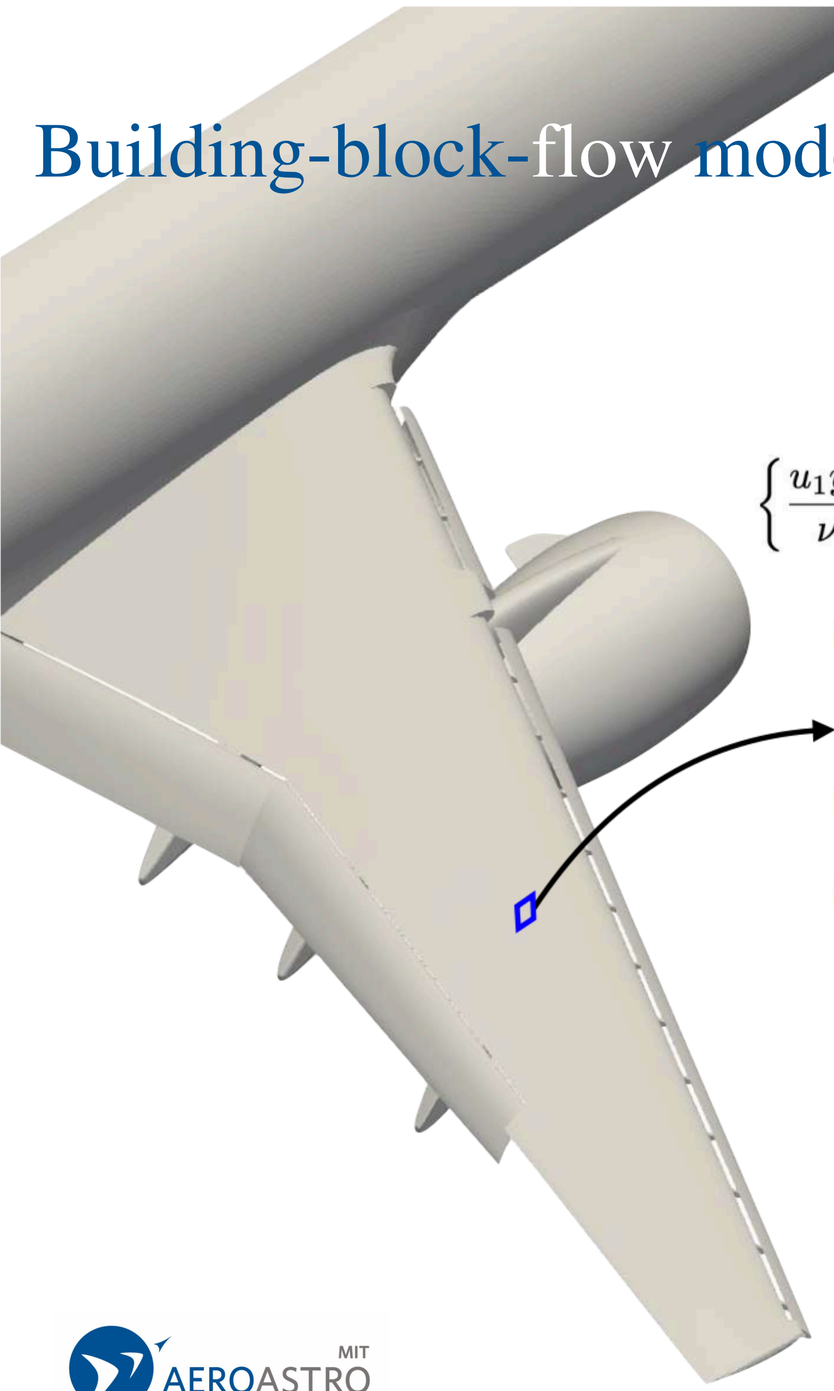
Adverse/favorable-pressure gradient (APG/FPG)
(Turbulent Poiseuille-Couette flow)

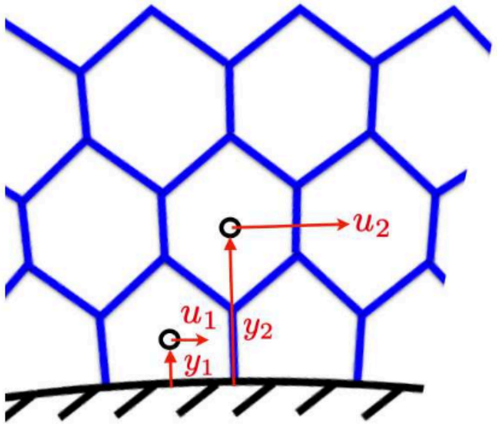


Strong unsteadiness and 3-D mean flow (Unsteady)
(channel with sudden lateral force)

Multiple cases of each building block sweeping through the non-dimensional groups

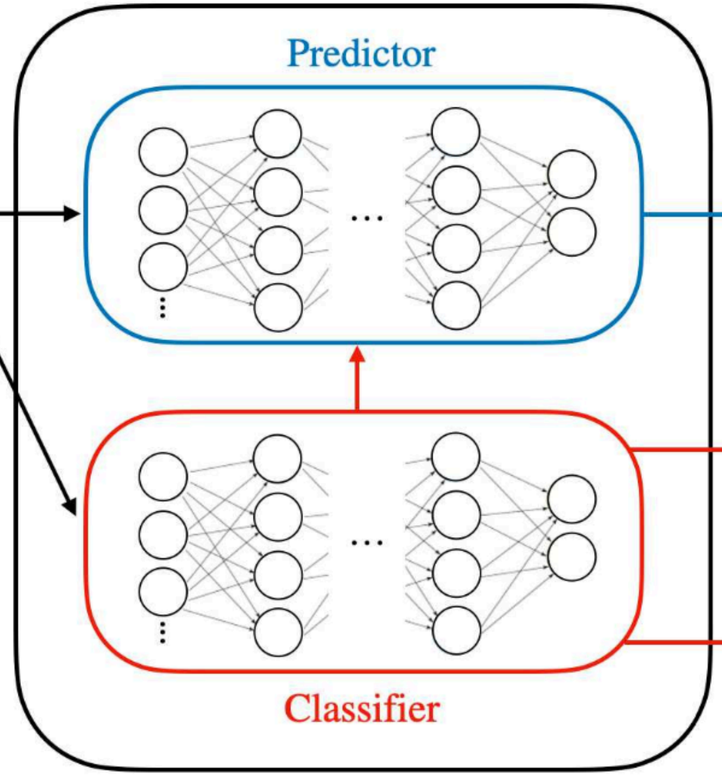
Building-block-flow model: architecture





Inputs

$$\left\{ \frac{u_1 y_1}{\nu}, \frac{u_2 y_2}{\nu}, \gamma_{12}, \frac{a_1 y_1^3}{\nu^2}, \frac{\dot{\gamma}_1 y_1^2}{\nu}, \frac{k_1}{k_{m1}} \right\}$$



Outputs

$$\left\{ \frac{\tau_w y_1}{\mu u_1}, \gamma_{1w} \right\}$$

% Freestream
% Laminar flow
% Separation
% APG
% ZPG
% FPG
% Unsteady

% Confidence

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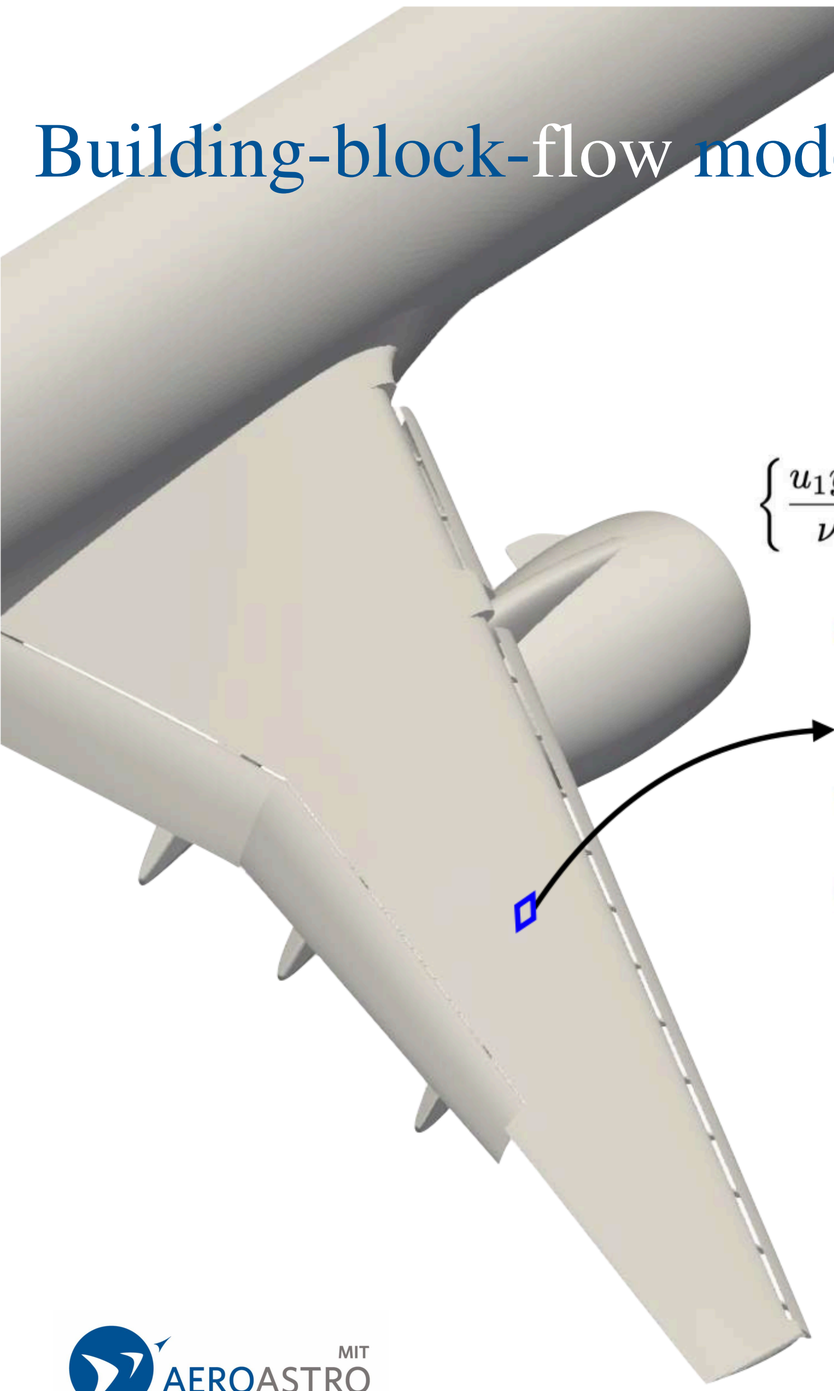
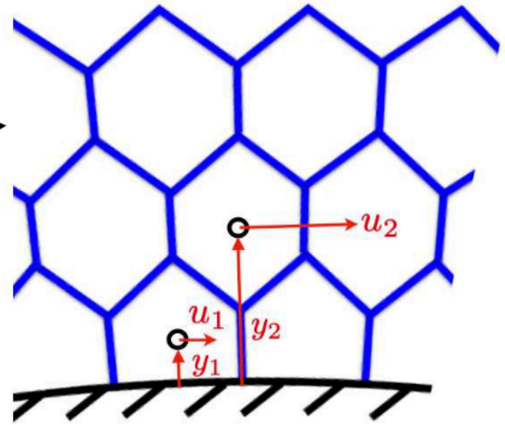
Building-block-flow model: architecture



Inputs

$$\left\{ \frac{u_1 y_1}{\nu}, \frac{u_2 y_2}{\nu}, \gamma_{12}, \frac{a_1 y_1^3}{\nu^2}, \frac{\dot{\gamma}_1 y_1^2}{\nu}, \frac{k_1}{k_{m1}} \right\}$$



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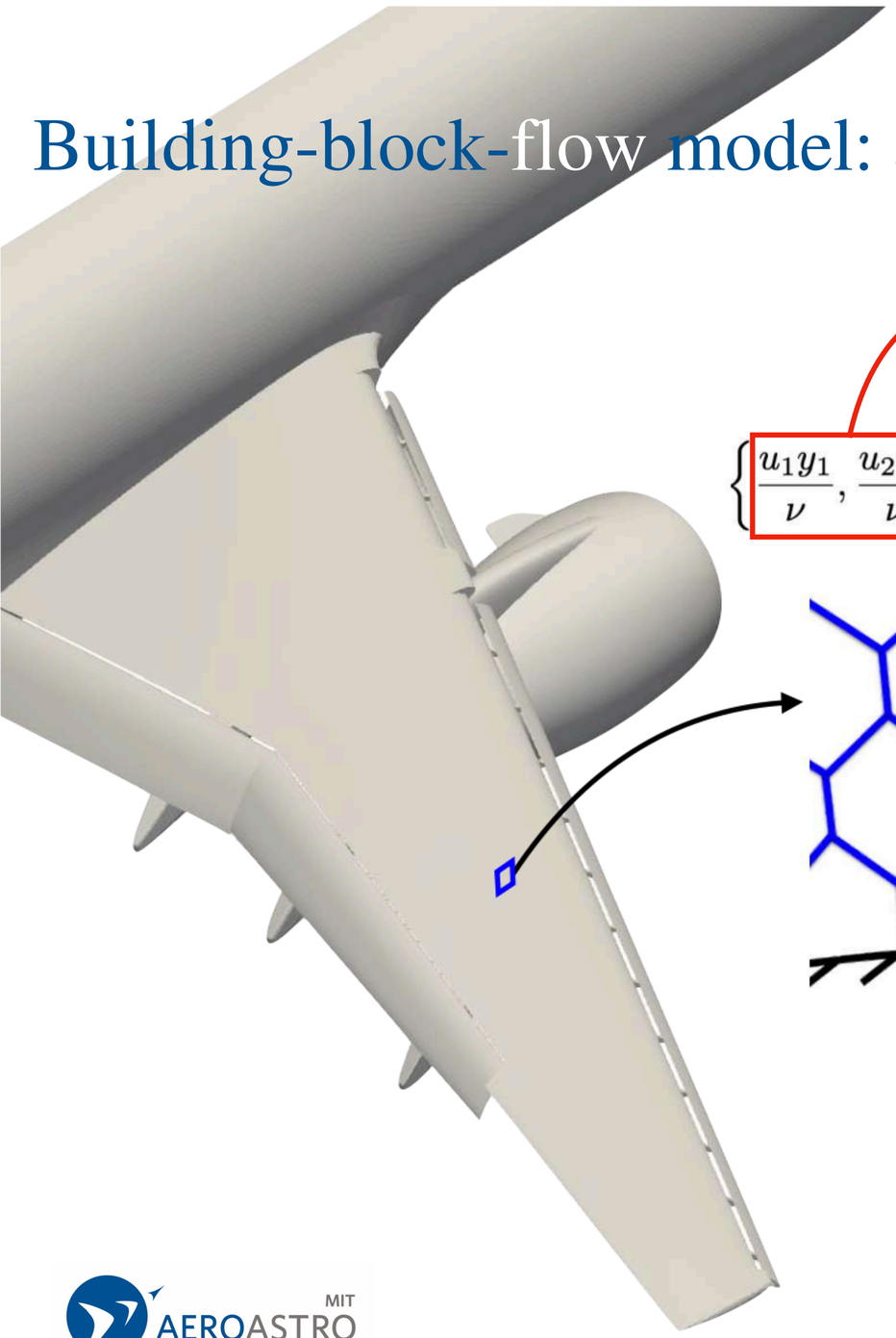
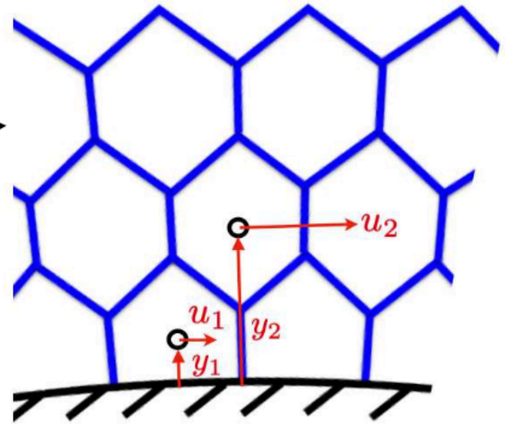
Building-block-flow model: architecture



Local Re: detect shape of the profile

Inputs

$$\left\{ \frac{u_1 y_1}{\nu}, \frac{u_2 y_2}{\nu}, \gamma_{12}, \frac{a_1 y_1^3}{\nu^2}, \frac{\dot{\gamma}_1 y_1^2}{\nu}, \frac{k_1}{k_{m1}} \right\}$$



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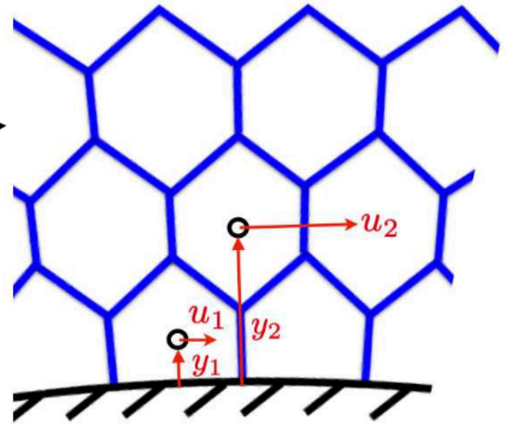
Building-block-flow model: architecture

Relative angle between velocities: 3-D effects

Inputs

$$\left\{ \frac{u_1 y_1}{\nu}, \frac{u_2 y_2}{\nu}, \gamma_{12}, \frac{a_1 y_1^3}{\nu^2}, \frac{\dot{\gamma}_1 y_1^2}{\nu}, \frac{k_1}{k_{m1}} \right\}$$



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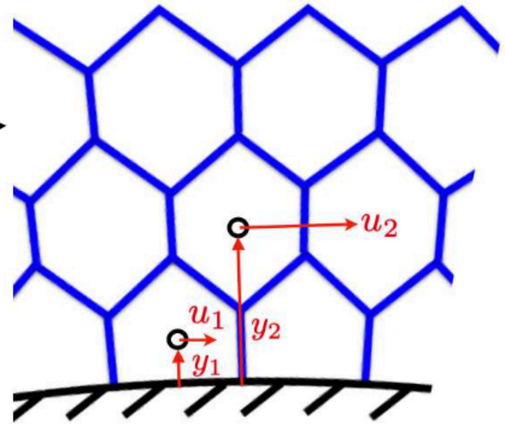
Building-block-flow model: architecture

Accelerations: unsteady effects

Inputs

$$\left\{ \frac{u_1 y_1}{\nu}, \frac{u_2 y_2}{\nu}, \gamma_{12}, \frac{a_1 y_1^3}{\nu^2}, \frac{\dot{\gamma}_1 y_1^2}{\nu}, \frac{k_1}{k_{m1}} \right\}$$



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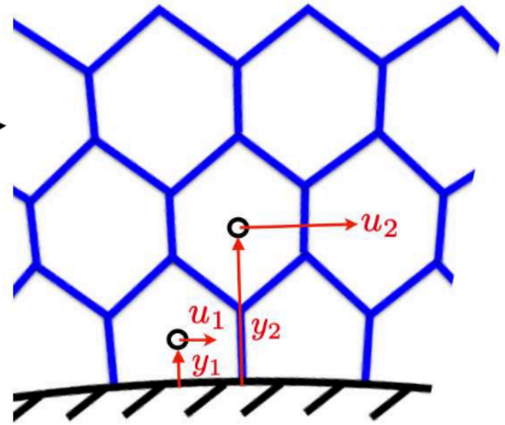
Building-block-flow model: architecture

Relative turbulent kinetic energy: laminar vs. turbulent

Inputs

$$\left\{ \frac{u_1 y_1}{\nu}, \frac{u_2 y_2}{\nu}, \gamma_{12}, \frac{a_1 y_1^3}{\nu^2}, \frac{\dot{\gamma}_1 y_1^2}{\nu}, \boxed{\frac{k_1}{k_{m1}}} \right\}$$



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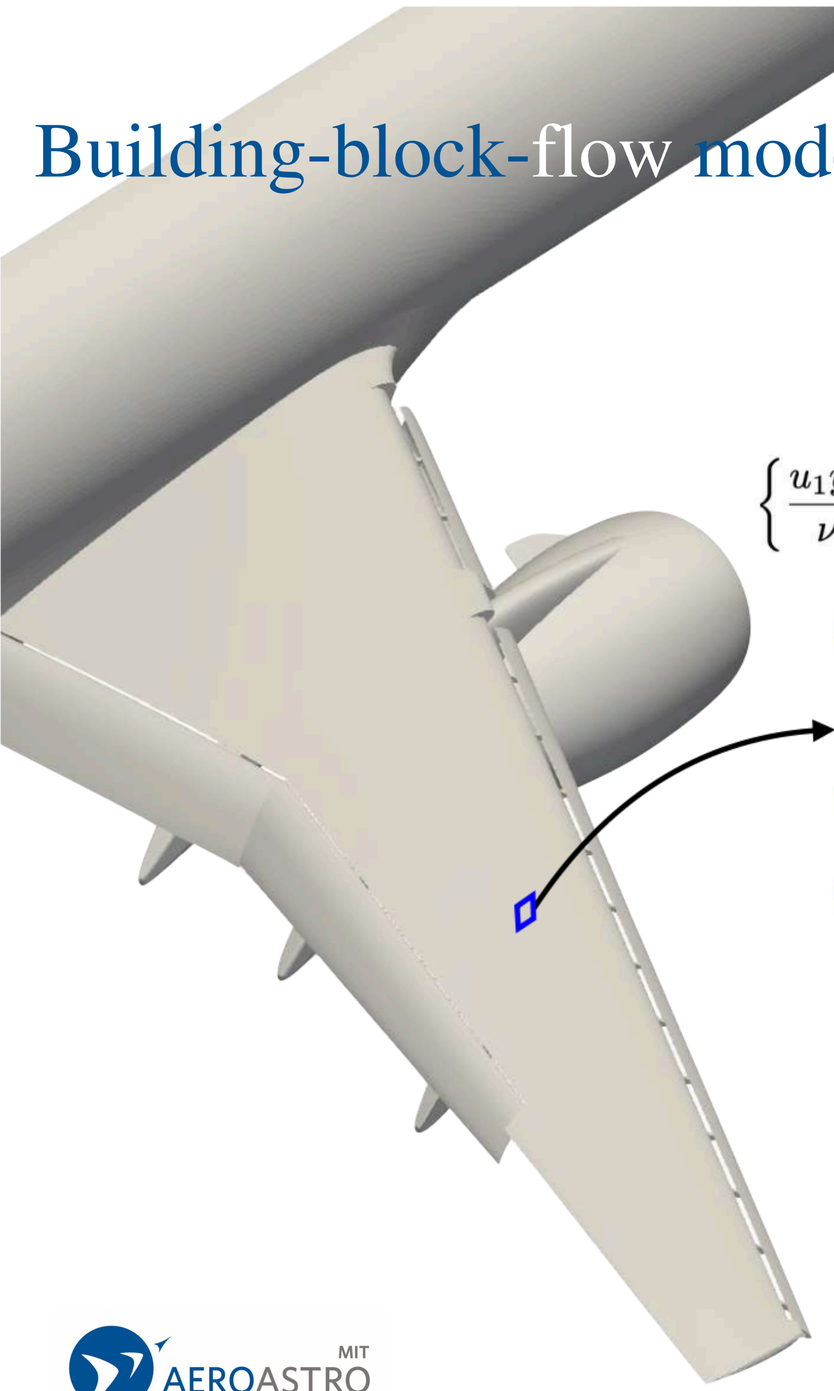
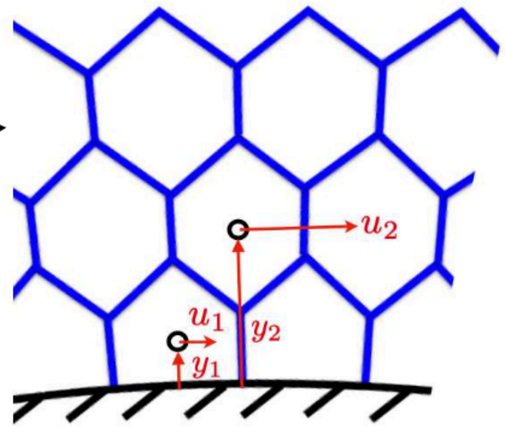
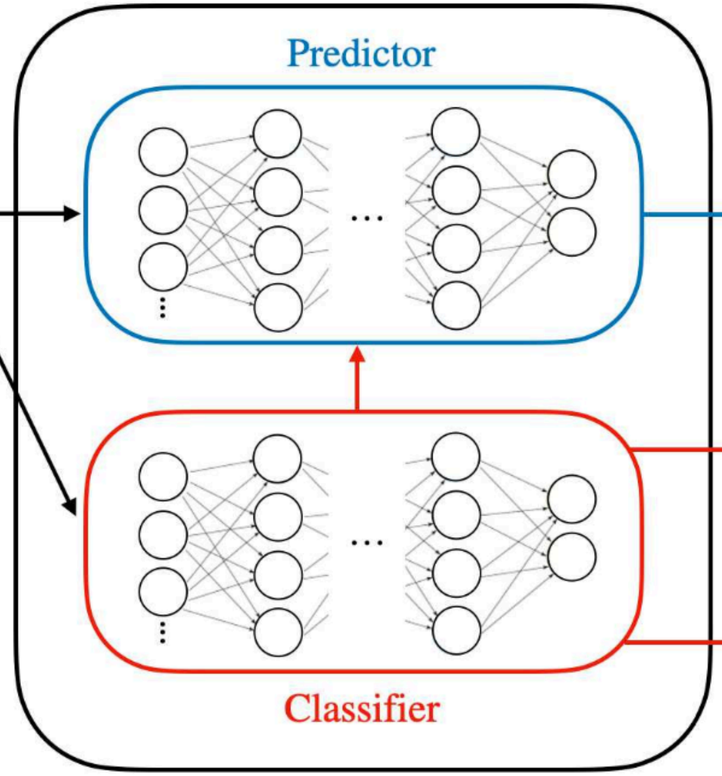
Building-block-flow model: architecture





Inputs

$$\left\{ \frac{u_1 y_1}{\nu}, \frac{u_2 y_2}{\nu}, \gamma_{12}, \frac{a_1 y_1^3}{\nu^2}, \frac{\dot{\gamma}_1 y_1^2}{\nu}, \frac{k_1}{k_{m1}} \right\}$$



Outputs

$$\left\{ \frac{\tau_w y_1}{\mu u_1}, \gamma_{1w} \right\}$$

- % Freestream
- % Laminar flow
- % Separation
- % APG
- % ZPG
- % FPG
- % Unsteady
- % Confidence

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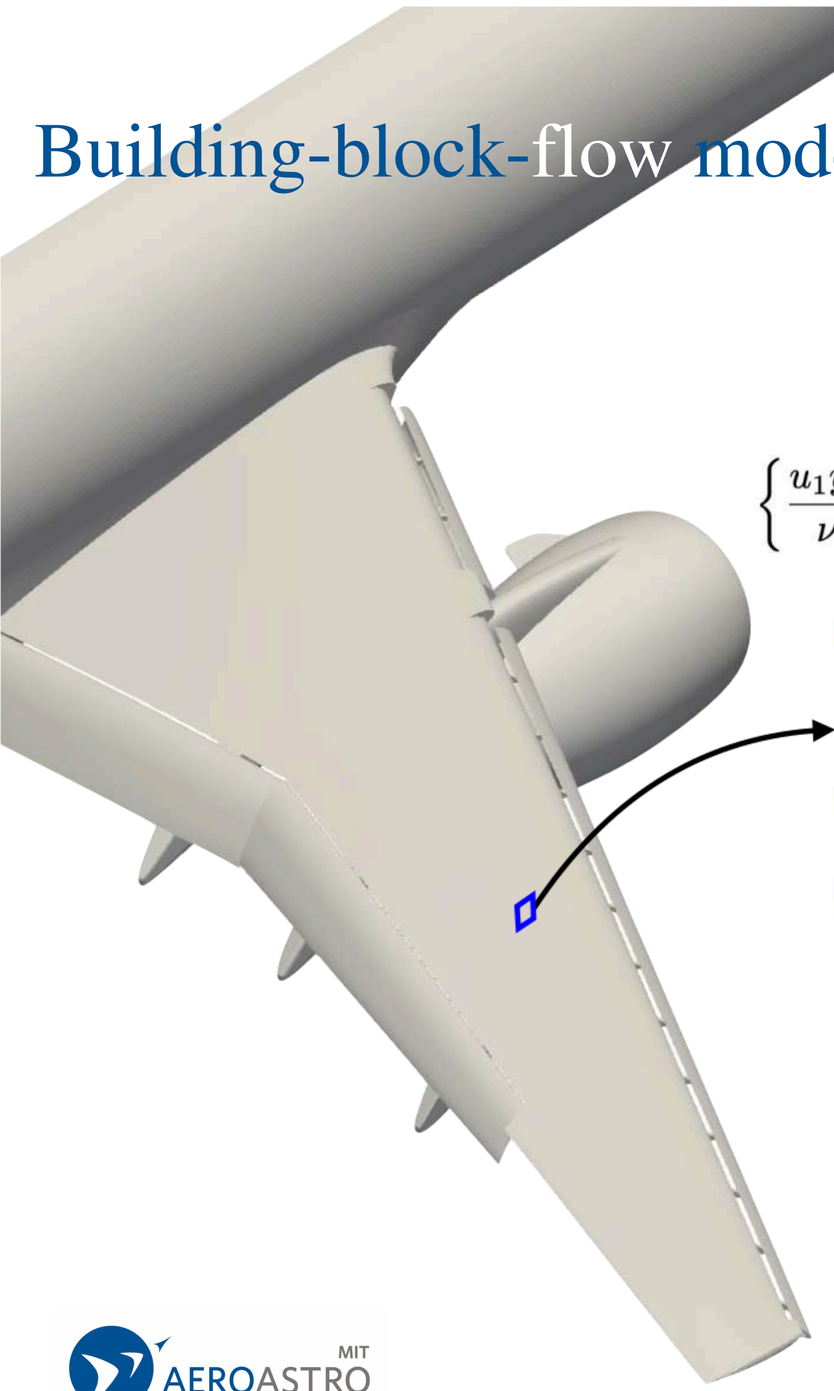
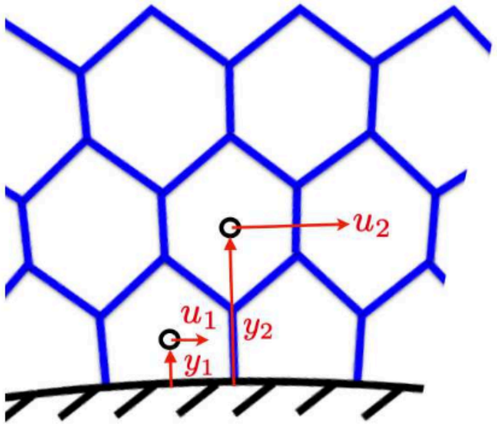
Building-block-flow model: architecture





Inputs

$$\left\{ \frac{u_1 y_1}{\nu}, \frac{u_2 y_2}{\nu}, \gamma_{12}, \frac{a_1 y_1^3}{\nu^2}, \frac{\dot{\gamma}_1 y_1^2}{\nu}, \frac{k_1}{k_{m1}} \right\}$$

Predictor

Classifier

Outputs

$$\left\{ \frac{\tau_w y_1}{\mu u_1}, \gamma_{1w} \right\}$$

Relative angles wall-stress vs. velocity 1

Wall-stress magnitude

% Freestream
% Laminar flow
% Separation
% APG
% ZPG
% FPG
% Unsteady

% Confidence

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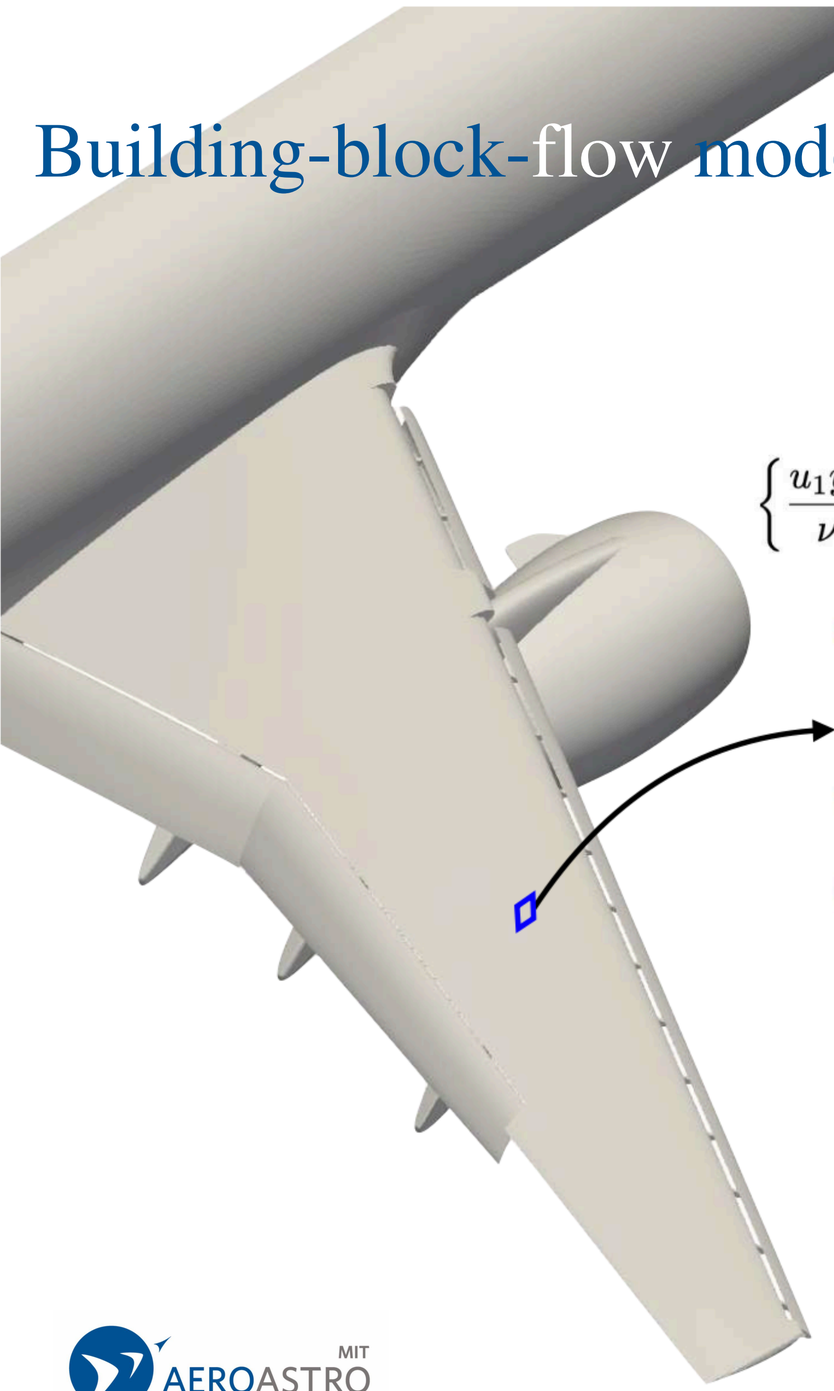
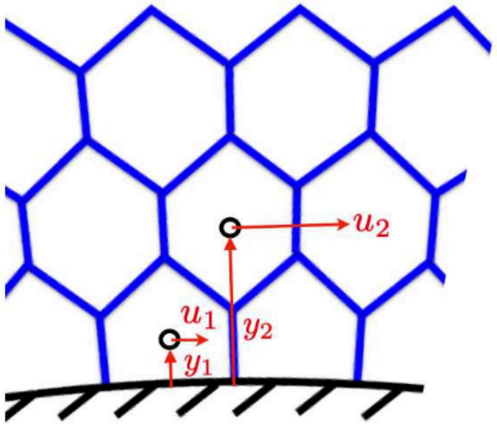
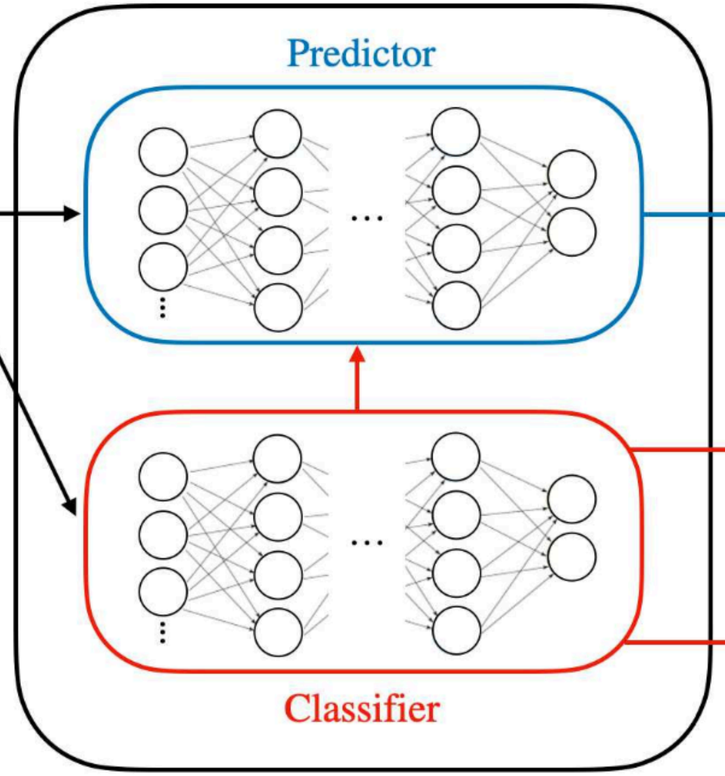
Building-block-flow model: architecture





Inputs

$$\left\{ \frac{u_1 y_1}{\nu}, \frac{u_2 y_2}{\nu}, \gamma_{12}, \frac{a_1 y_1^3}{\nu^2}, \frac{\dot{\gamma}_1 y_1^2}{\nu}, \frac{k_1}{k_{m1}} \right\}$$



Outputs

$$\left\{ \frac{\tau_w y_1}{\mu u_1}, \gamma_{1w} \right\}$$

% Freestream
% Laminar flow
% Separation
% APG
% ZPG
% FPG
% Unsteady

p^i_{class}

% Confidence

- Predictor: Deep feedforward NN, 5 hidden layers, 30 neurons per layer
- Classifier: Bayesian NN, 5 hidden layers, 20 neurons per layer
- Confidence score based on how close the input data is to the training set

Predictions: $\tau_w = \sum_{i=1}^{7} \tau_w^i p^i_{\text{class}} \qquad \gamma_{1w} = \sum_{i=1}^{7} \gamma_{1w}^i p^i_{\text{class}}$

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Building-block-flow model: training data

The training data is obtained by performing WMLES with exact-for-the-mean SGS/wall model

- A pseudo-SGS/wall model with knowledge of DNS solution is implemented in the WMLES solver
- This enforces consistency of the building-block model with the numerical schemes

Flow solver: charLES (from Cascade Tech. & Stanford)

- Second order finite volume
- 3rd order Runge-Kutta time-stepping
- Voronoi grid

Building-block-flow model: training data

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Flow solver: charLES (from Cascade Tech. & Stanford)

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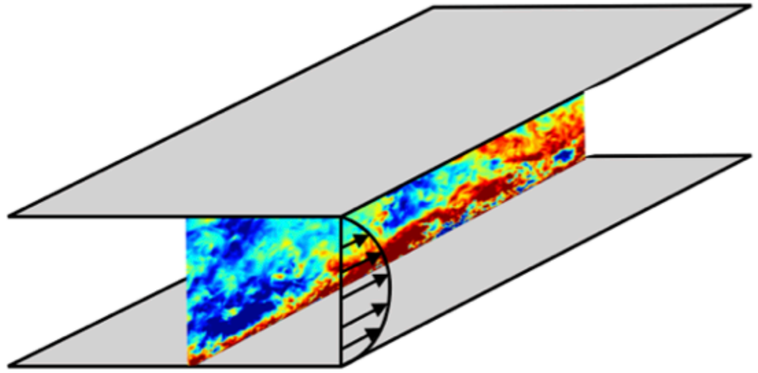
DNS
Mean velocity profiles
and wall stress p.d.f.



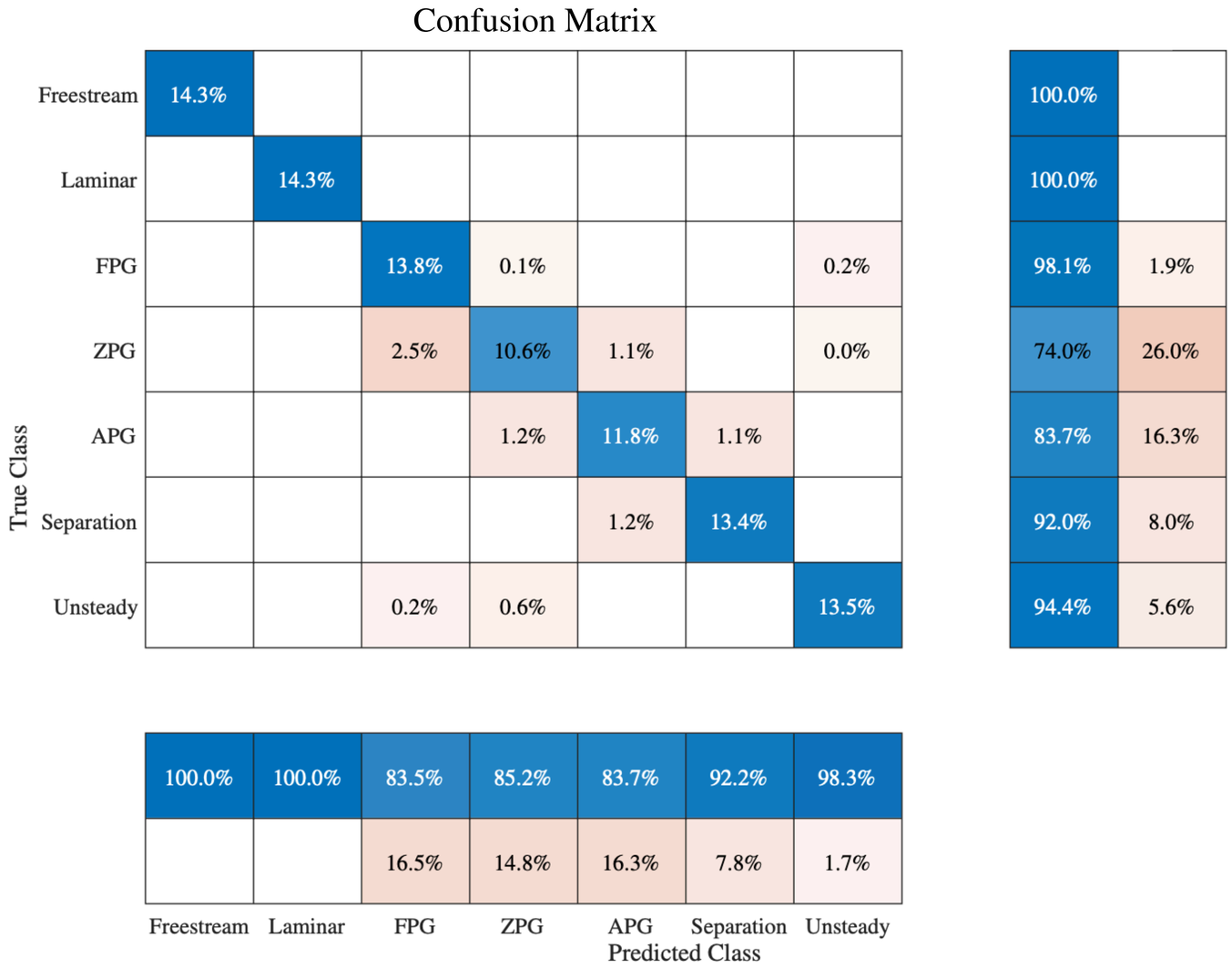
Training data

WMLES with an SGS/wall model matches DNS mean velocity profiles and wall stress accounting for numerical errors and gridding strategy

Building-block-flow model: classifier performance

Diagonal:
- Samples correctly classified

Off-diagonal:
- Samples misclassified



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Validation Case I:
NASA Juncture flow

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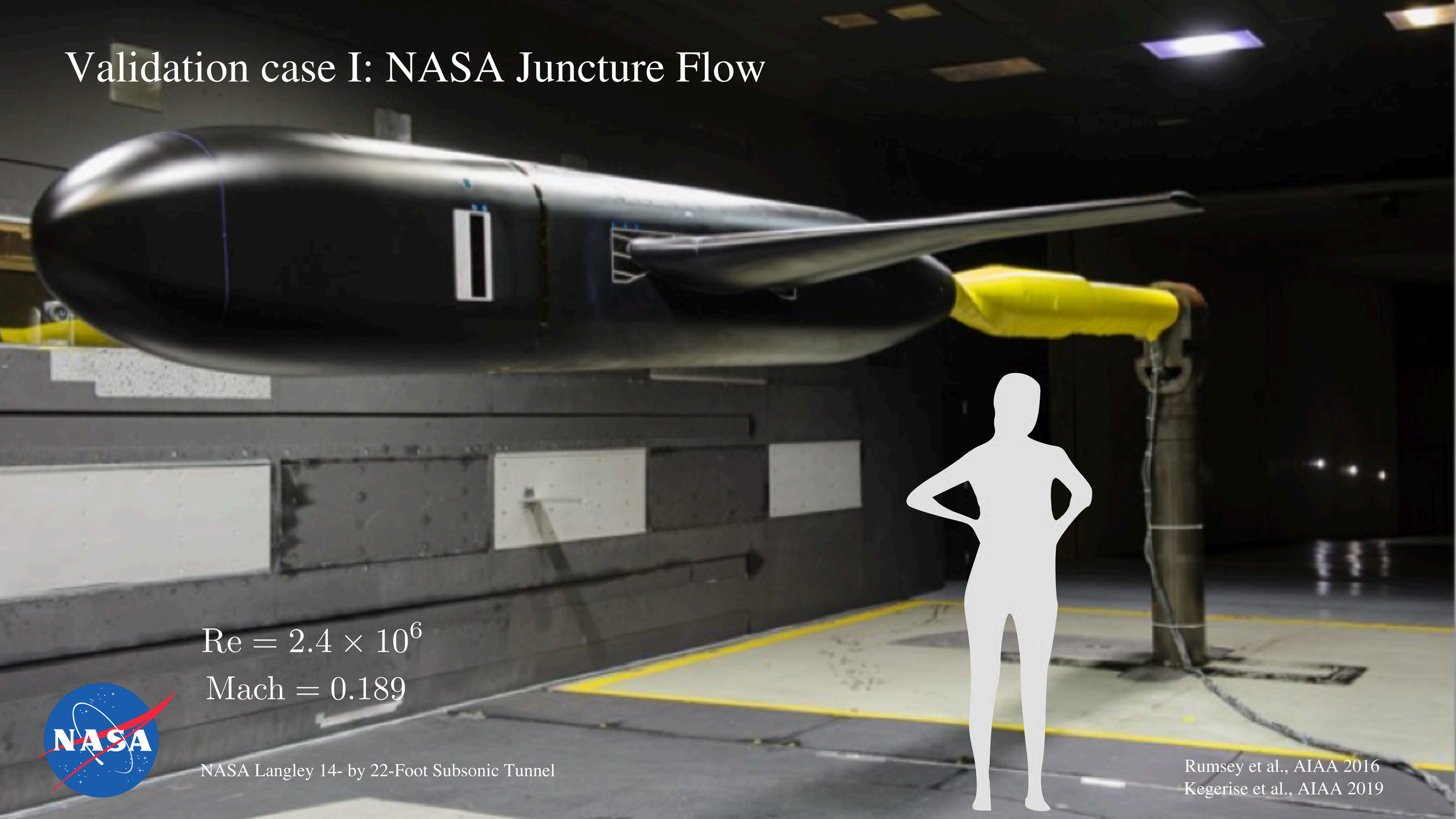
Validation case I: NASA Juncture Flow



$$\mathrm{Re} = 2.4 \times 10^6$$

$$\mathrm{Mach} = 0.189$$

NASA Langley 14- by 22-Foot Subsonic Tunnel

Rumsey et al., AIAA 2016
Kegerise et al., AIAA 2019

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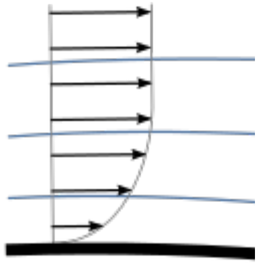
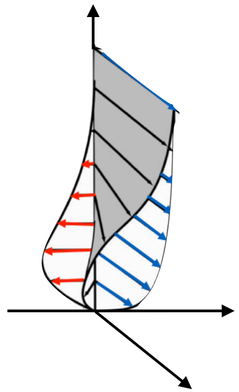
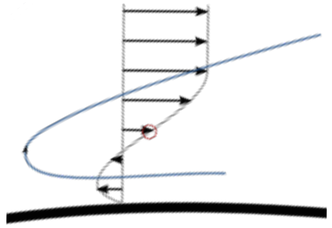


~Zero-pressure gradient turbulent boundary layer



Boundary layer with 3-D mean-flow

Separated flow + 3-D mean flow



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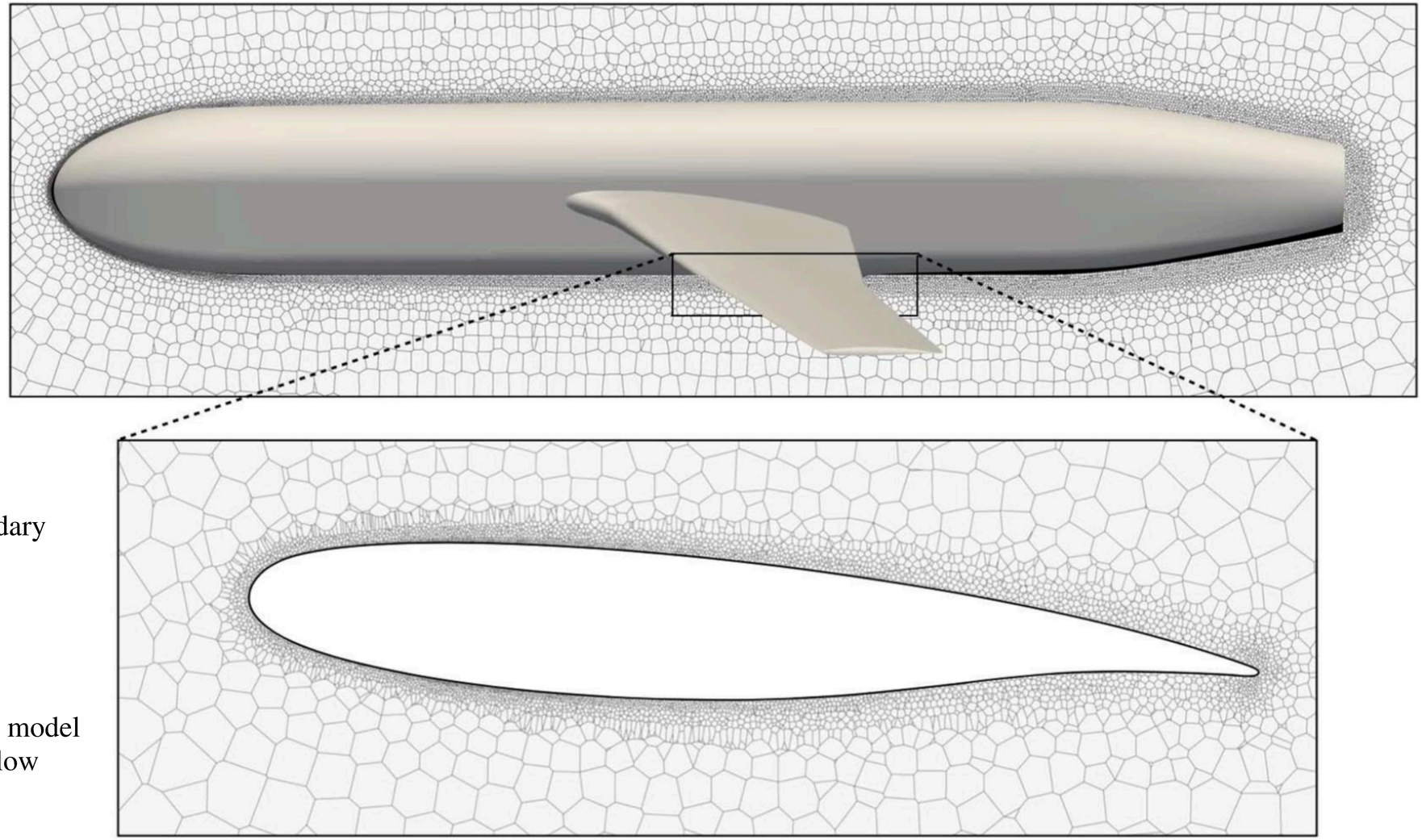

Grid resolution:

- 5 points per boundary layer thickness

Dynamic Smagorinsky

Wall models:

- Equilibrium wall model
- Building-block flow

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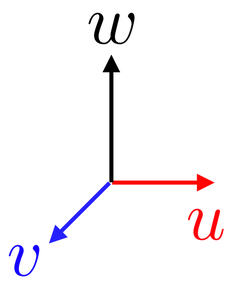
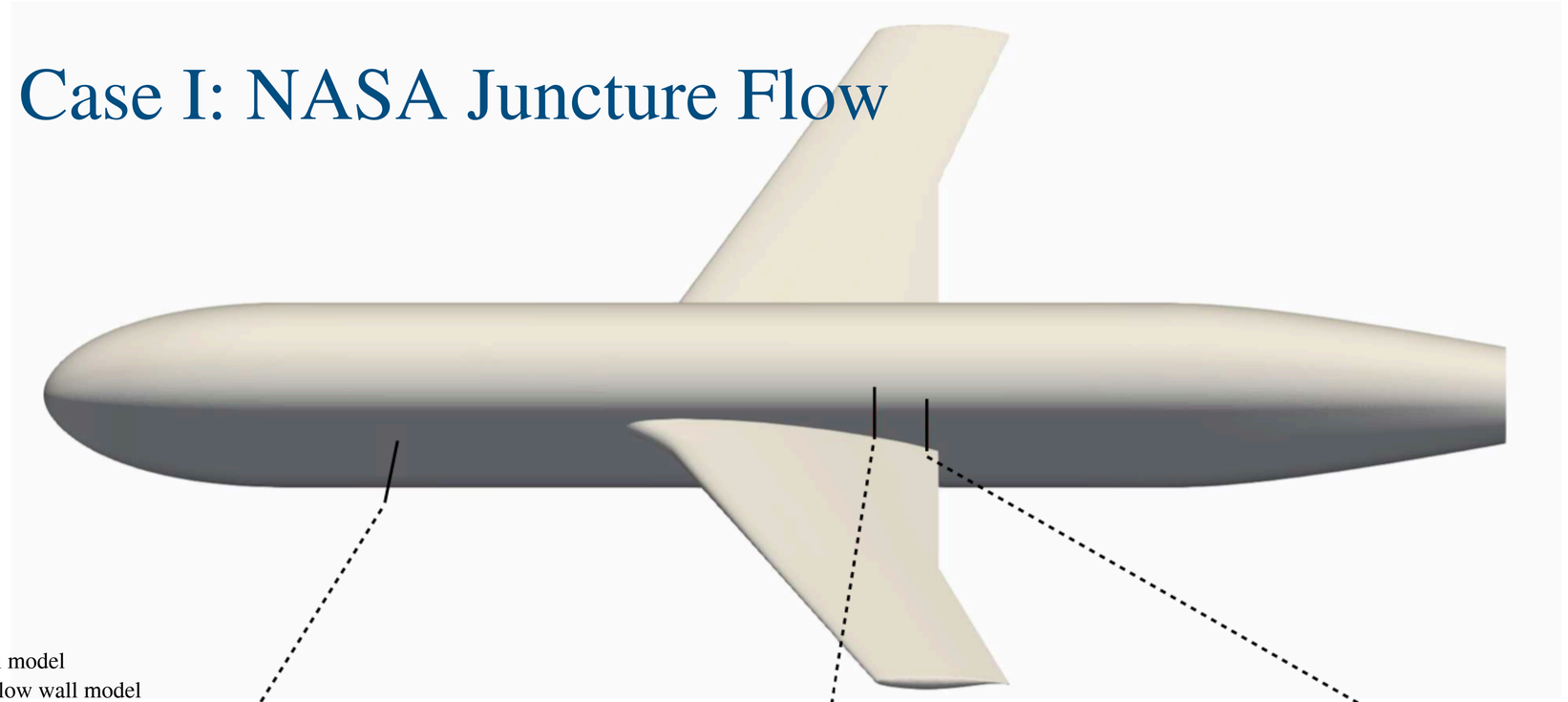
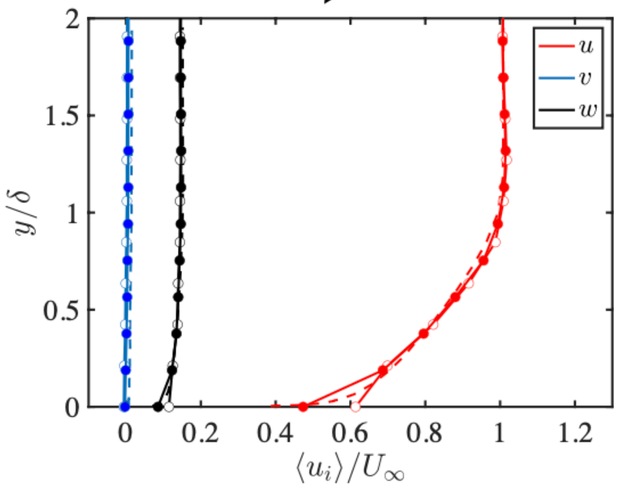
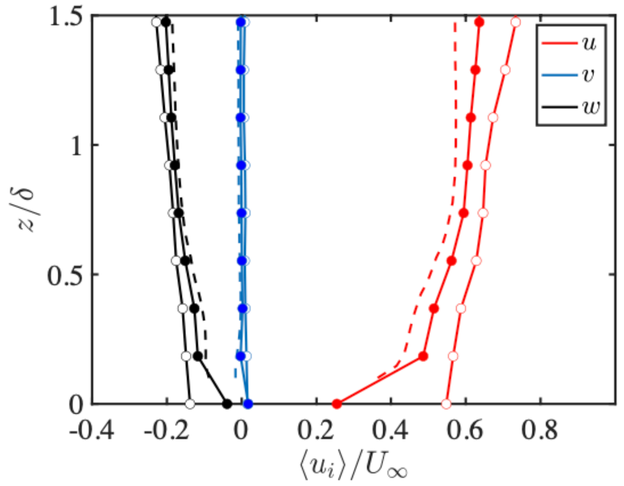
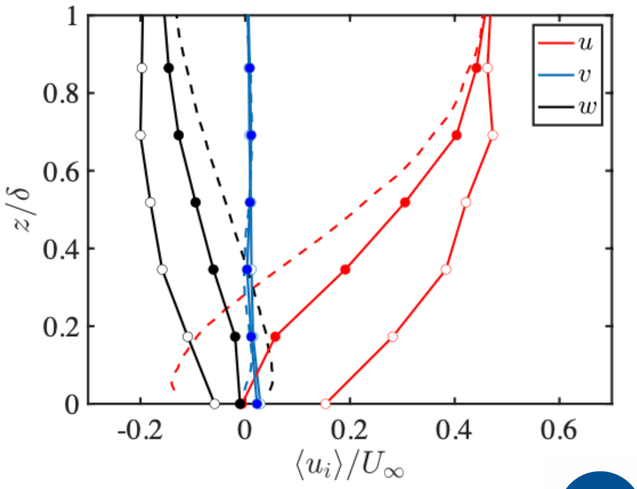




Equilibrium wall model
Building-block flow wall model







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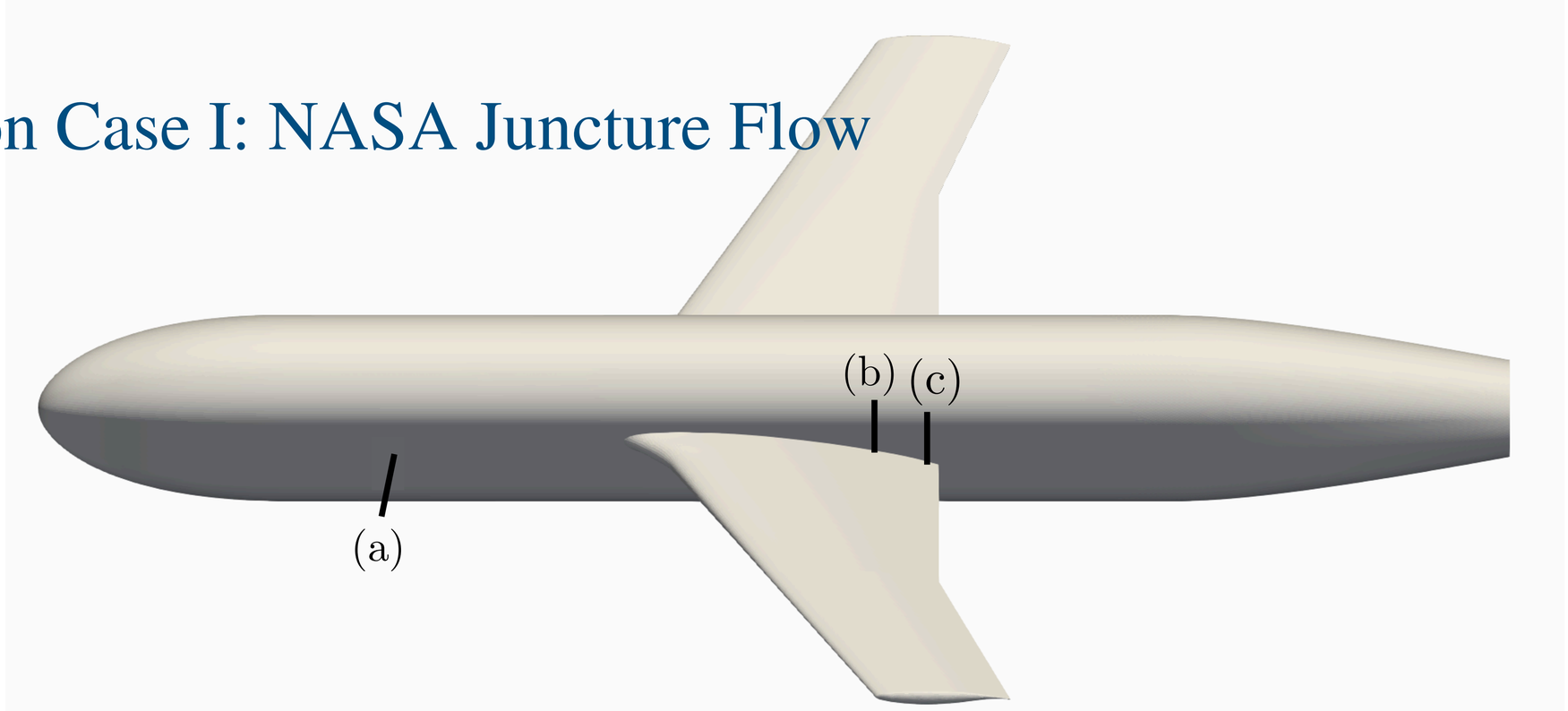

		Location (a)	Location (b)	Location (c)
Classification	Freestream	0%	0%	0%
	Laminar	0%	0%	0%
	FPG	12%	0%	0%
	ZPG	88%	41%	13%
	APG	0%	52%	31%
	Separation	0%	7%	56%
	Unsteady	0%	0%	0%
Confidence		98%	82%	22%

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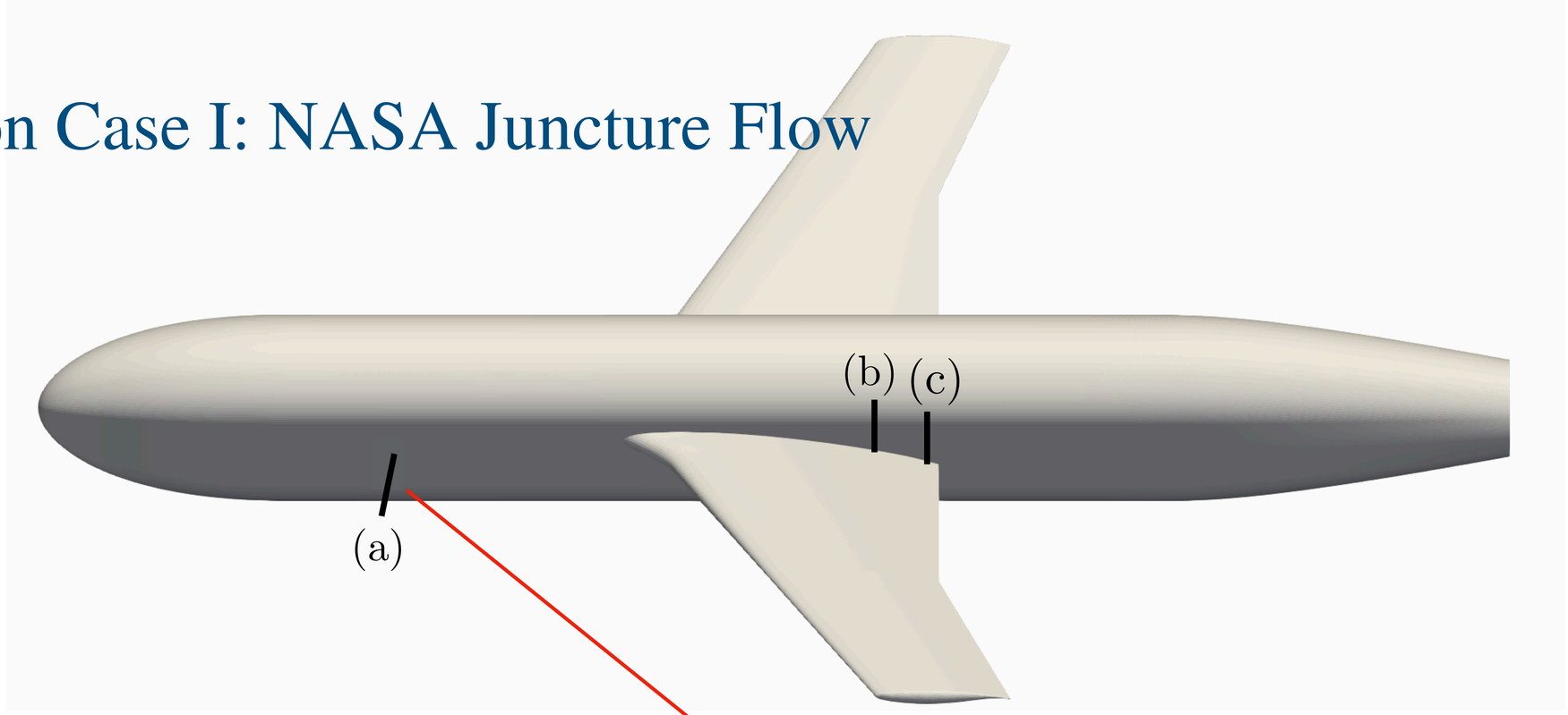

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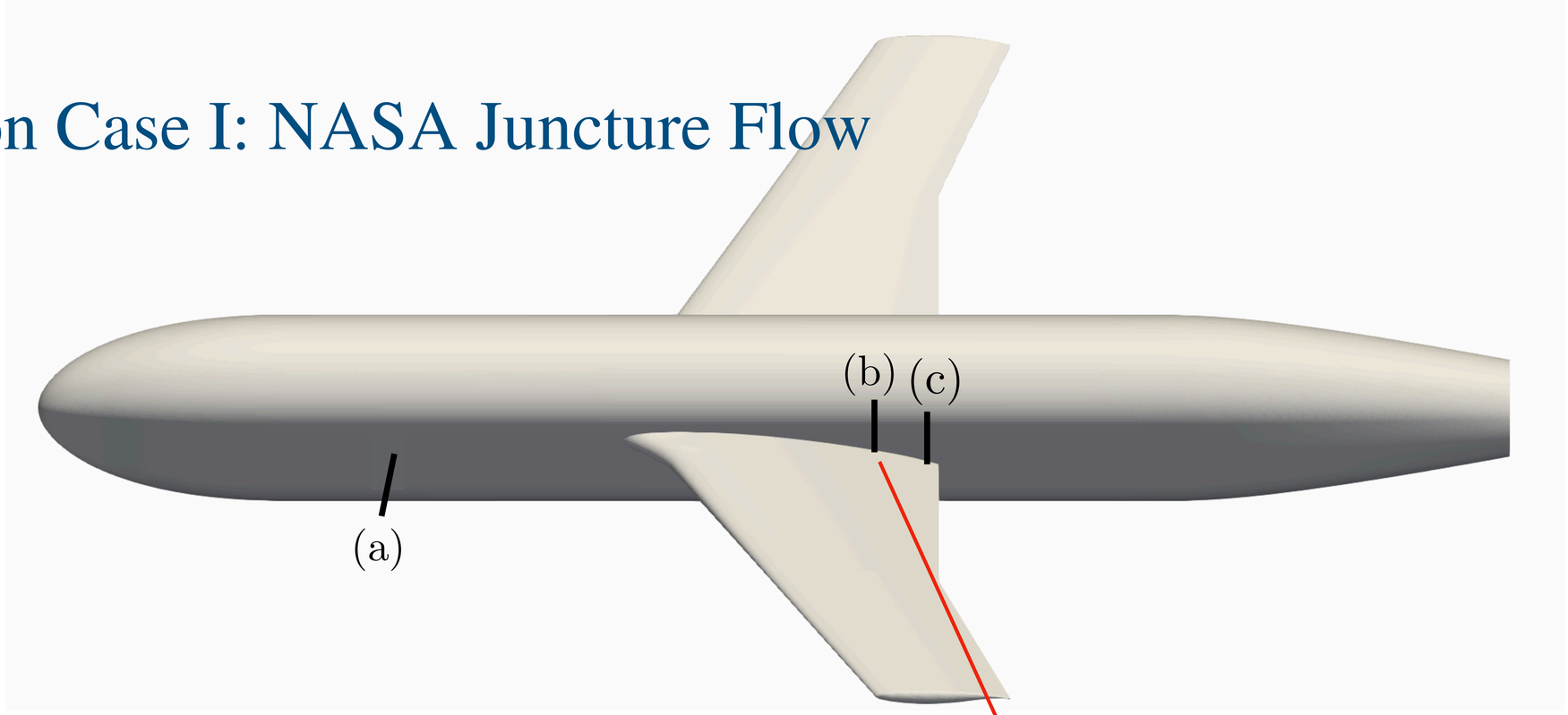

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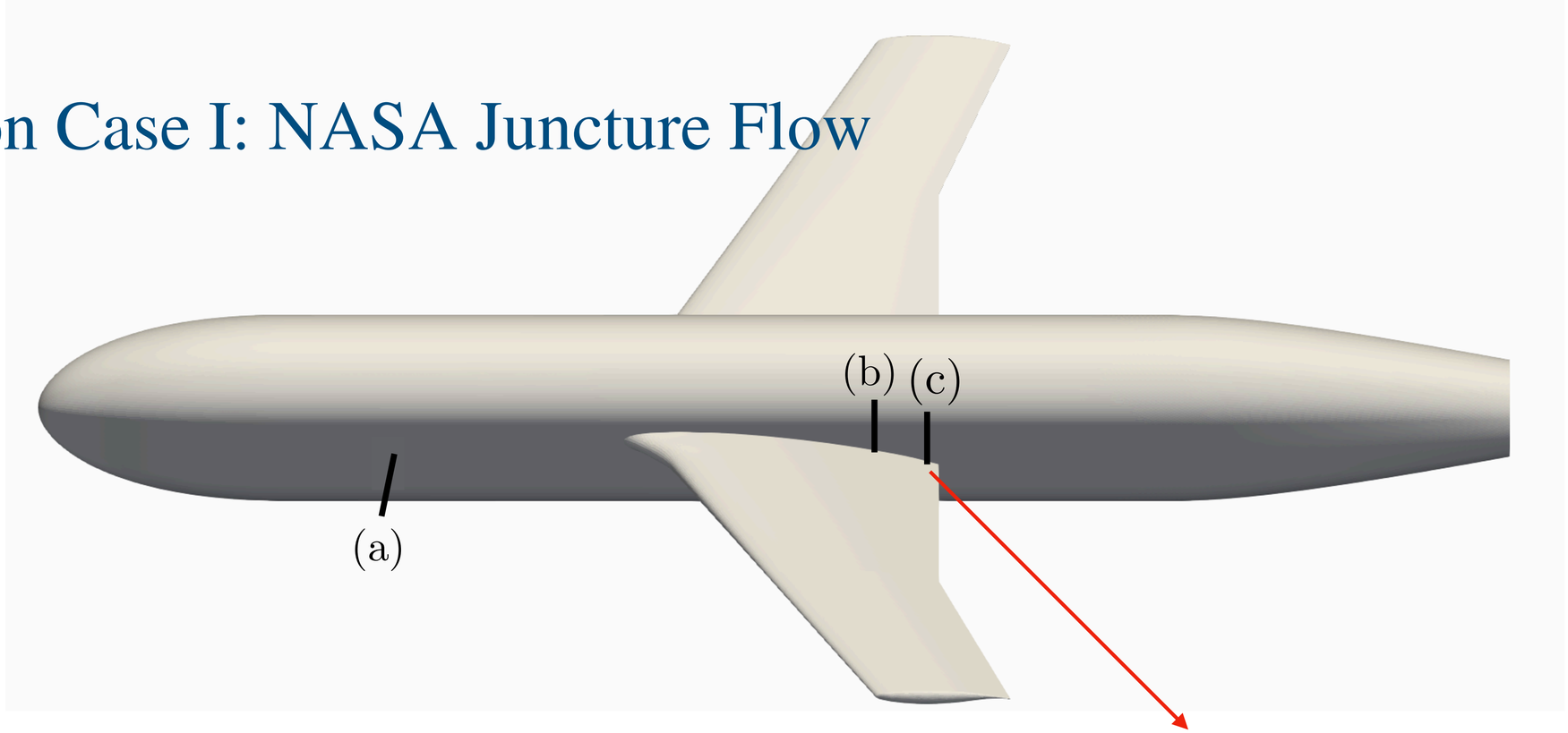

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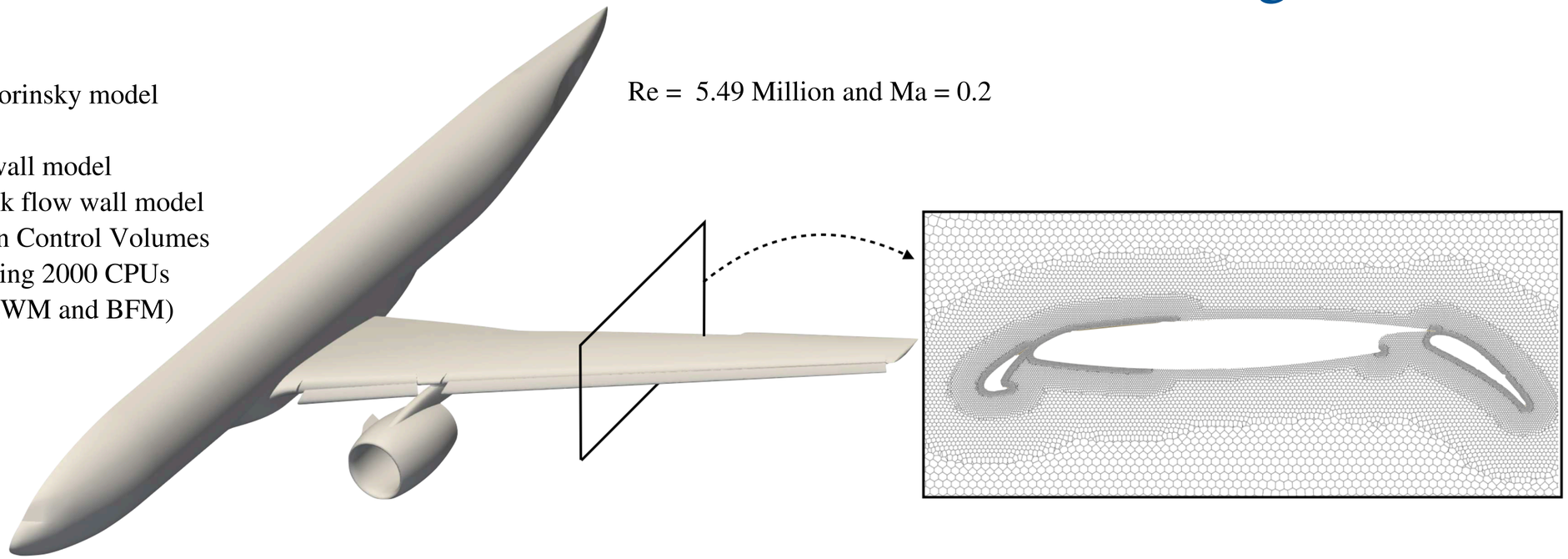
Validation Case II:
NASA Common Research Model High-Lift

Validation Case II: NASA Common Research Model High-Lift

- Dynamic Smagorinsky model
- Wall models:
  - Equilibrium wall model
  - Building-block flow wall model
- Grid: 30 Million Control Volumes
- Cost: ~1 day using 2000 CPUs
  (similar for EQWM and BFM)

Re = 5.49 Million and Ma = 0.2



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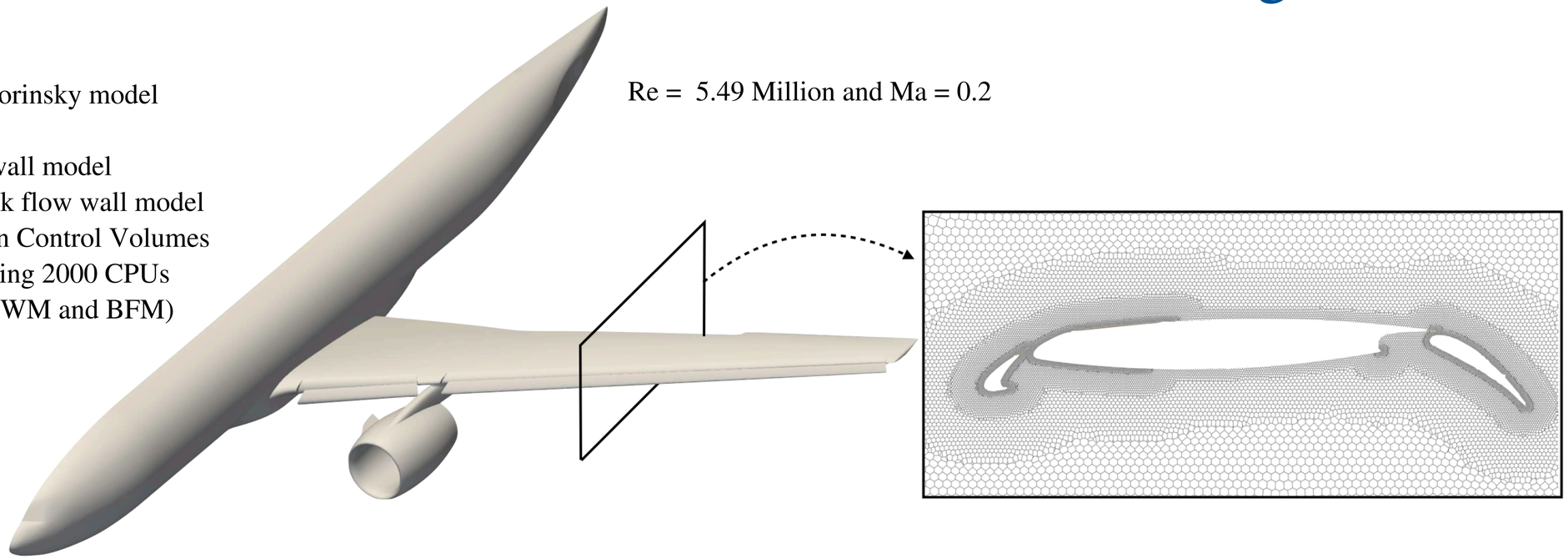
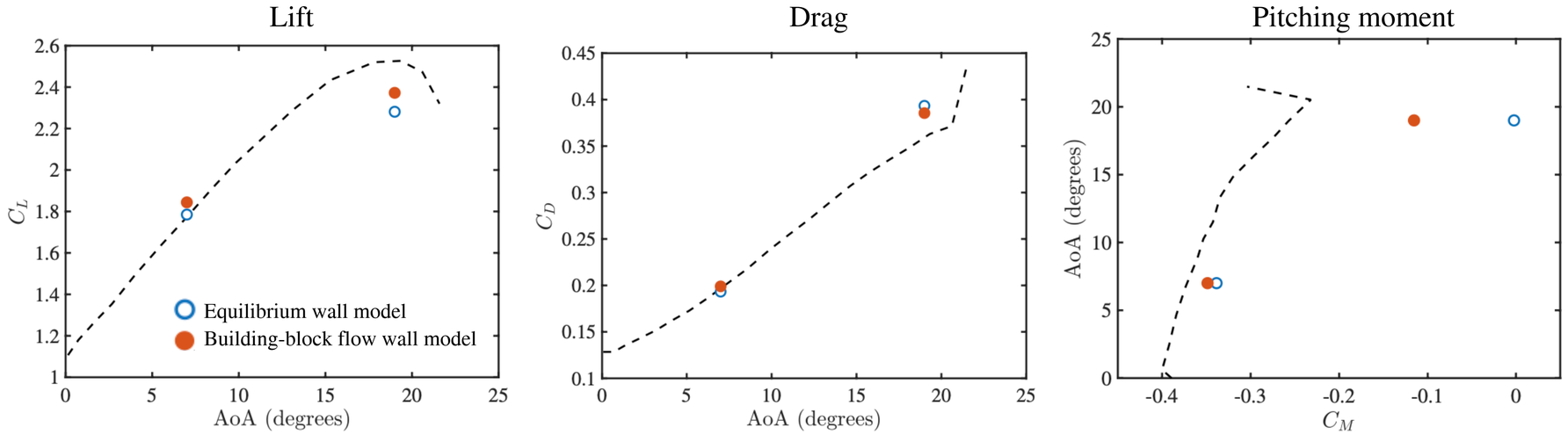
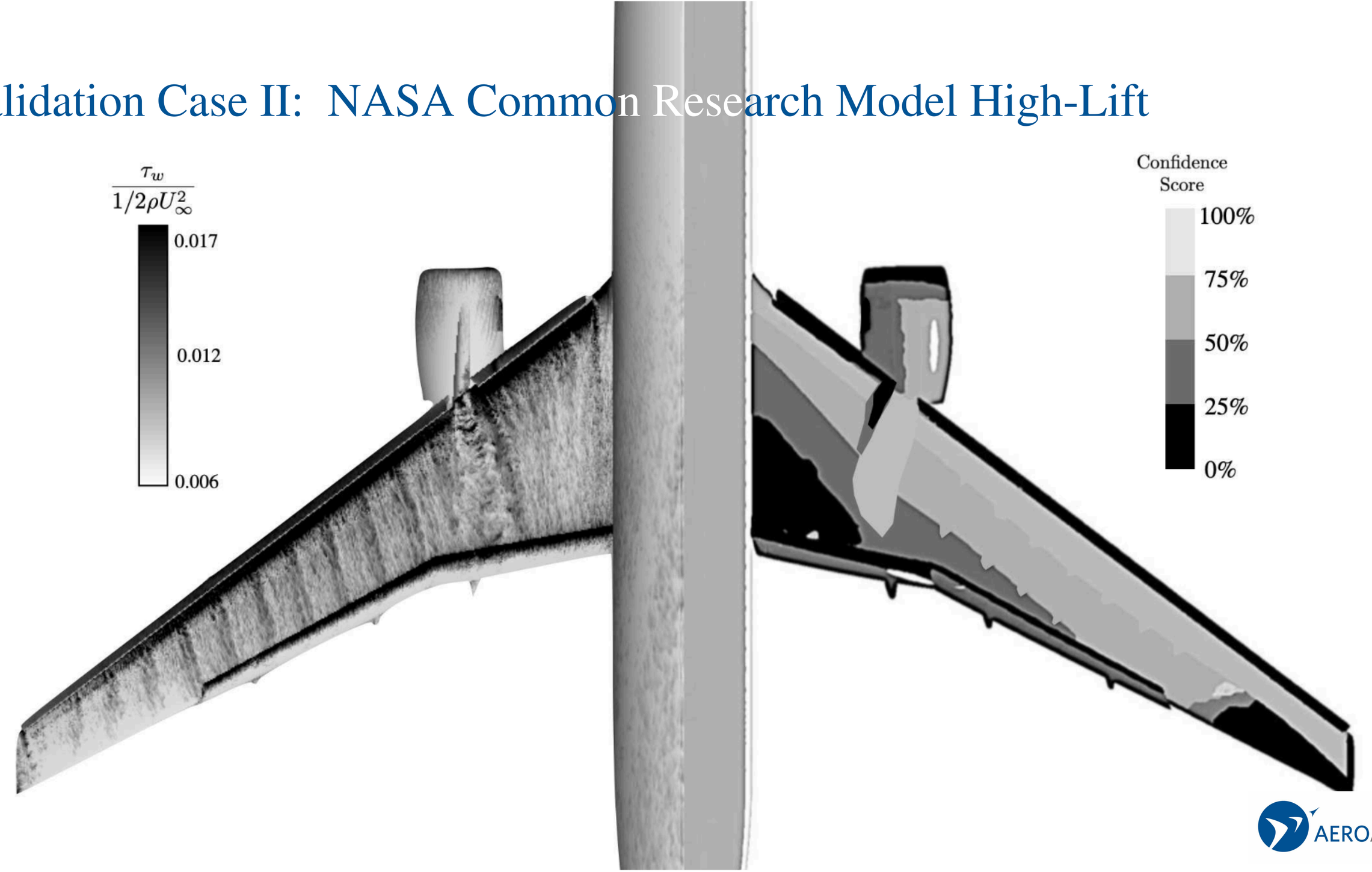




Validation Case II: NASA Common Research Model High-Lift



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Building-block flow model for SGS-model +wall-model

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Building-block flow model for SGS-model +wall-model

Center for Turbulence Research
Proceedings of the Summer Program 2022

Wall-modeled LES based on building-block flows

By Y. Ling†, G. Arranz†, E. Williams†, K. Goc, K. Griffin AND A. Lozano-Duran†

A unified subgrid-scale (SGS) and wall model for large-eddy simulation (LES) is proposed by devising the flow as a collection of building blocks that enables the prediction of the eddy viscosity. The core assumption of the model is that simple canonical flows contain the essential physics to provide accurate predictions in more complex flows. The model is constructed to predict zero-pressure-gradient wall-bounded turbulence, adverse pressure gradient effects, separation, and laminar flow. The approach is implemented using a Bayesian classifier, which identifies the contribution of each building block in the flow, and a neural-network-based predictor, which estimates the eddy viscosity based on the building-block units. The training data are directly obtained from wall-modeled LES with an exact SGS/wall model for the mean quantities to guarantee consistency with the numerical discretization. The model is validated in the NASA Common Research Model High-lift and shown to improve the predictions with respect to current modeling approaches.

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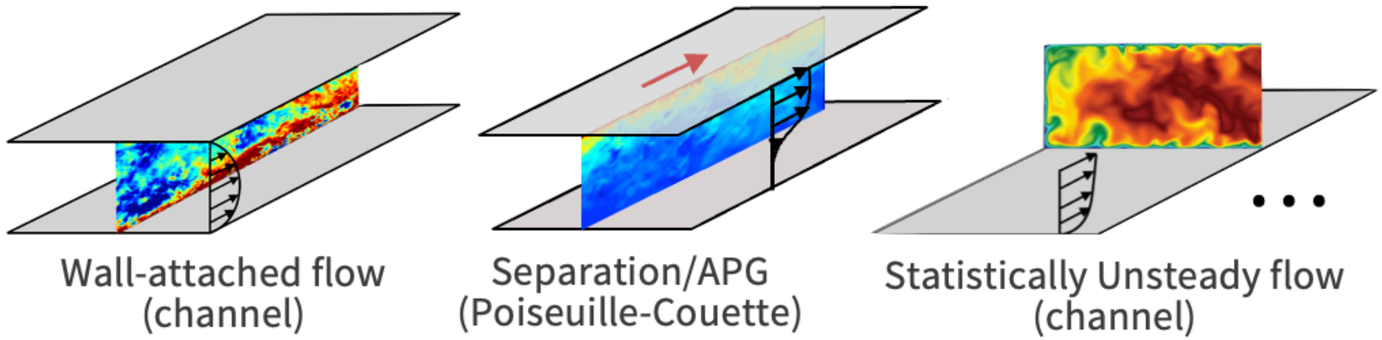
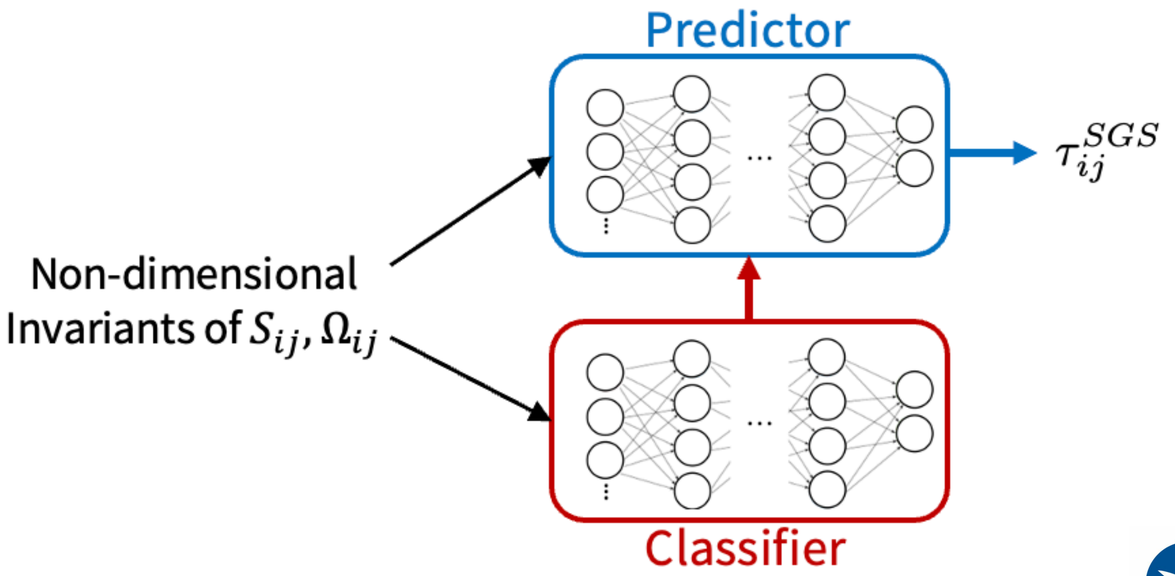
Building-block flow model for SGS-model +wall-model

Unified wall/SGS model:

- Accounting for different flows
  - laminar, APG, separation,…
- Compensating for numerical errors
- Applicable to complex geometries
- Accurate for typical WMLES resolutions
- Confidence score in the predictions

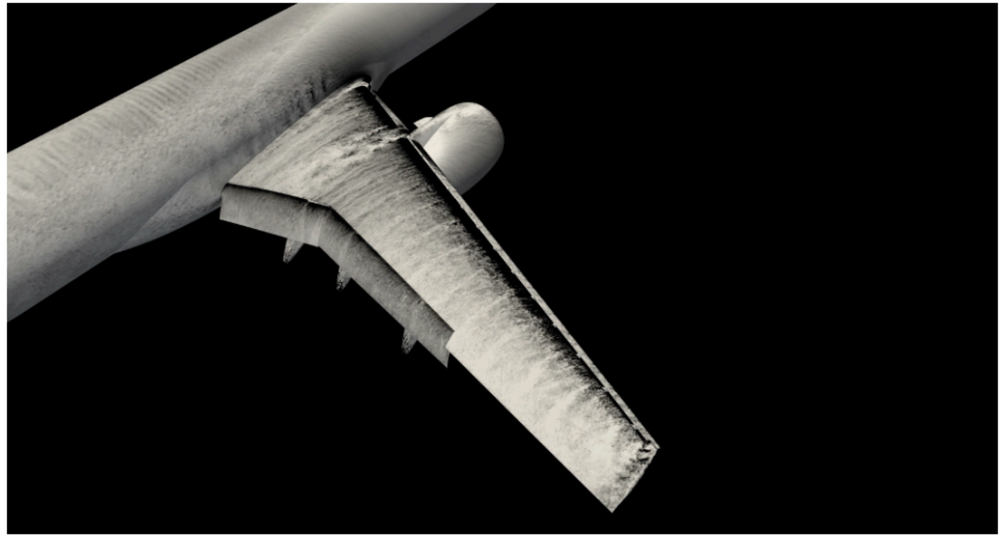


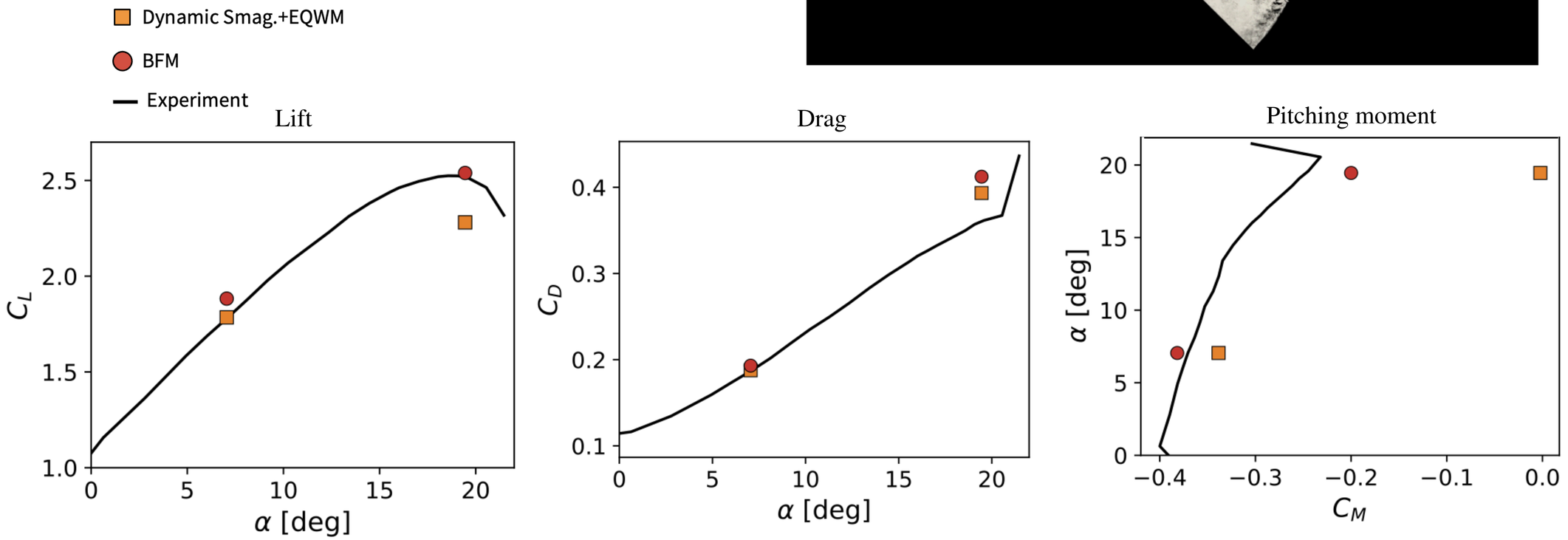


Ling et al. Proceedings of the CTR Summer Program 2022

Validation Case II revisited: NASA Common Research Model High-Lift

- Building-block flow model for SGS and wall (BFM)
- Dynamic Smagorinsky model + Equilibrium wall model (EQWM)
- Grid: 30 Million Control Volumes
- Cost of BFM is roughly x5 Dynamic Smag+EQWM
  - but no optimization attempted





Limitations

- What are the fundamental building blocks? How many?

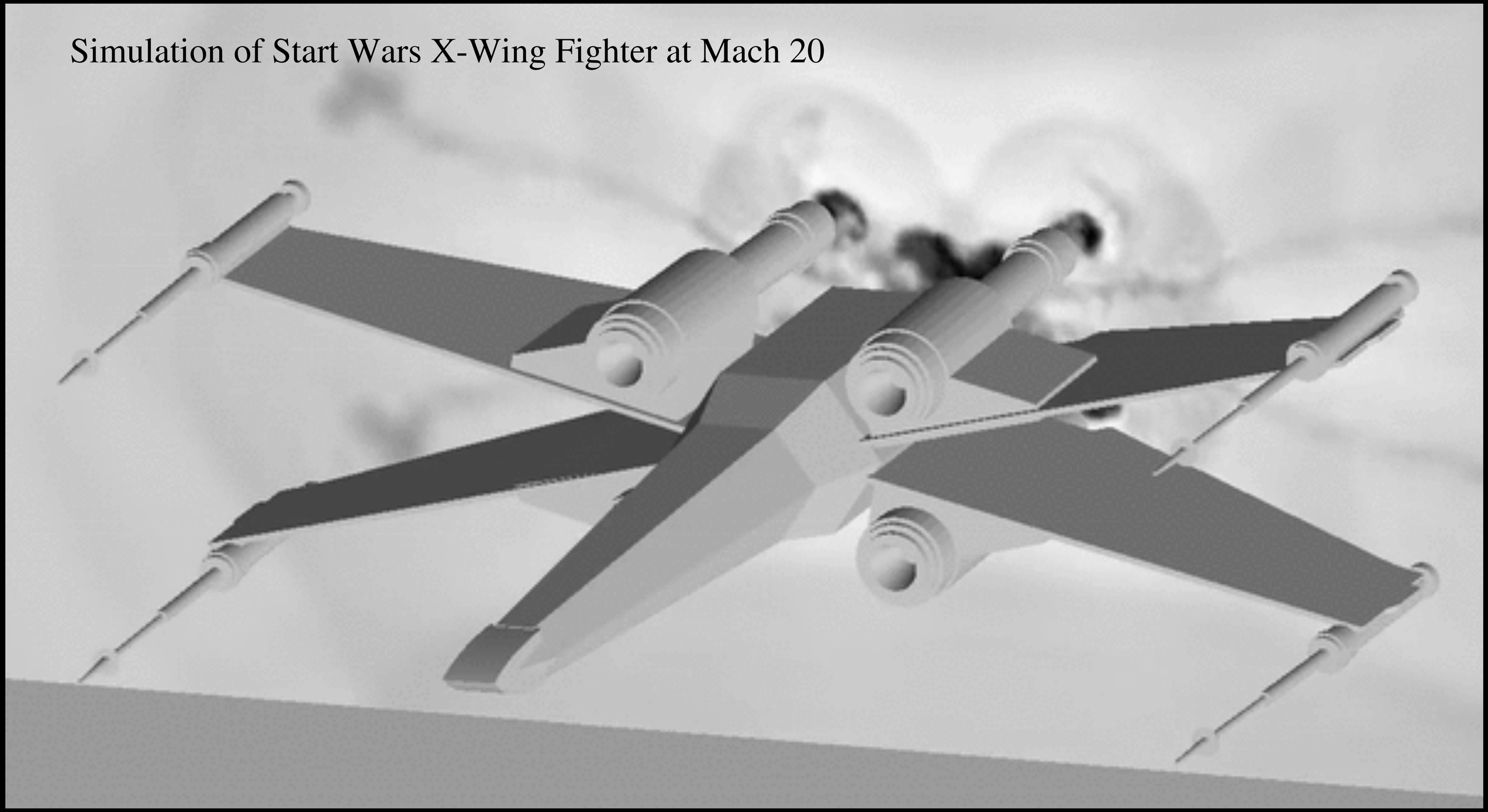
- Physics unaccounted for: compressibility effects, shock waves, chemical reactions, multiphase flows, different mean-flow three-dimensionalities and separation patterns,…

- The confidence score offered by BFM is based on the similarities between the input flow features and the building-block flows, not on the prediction.

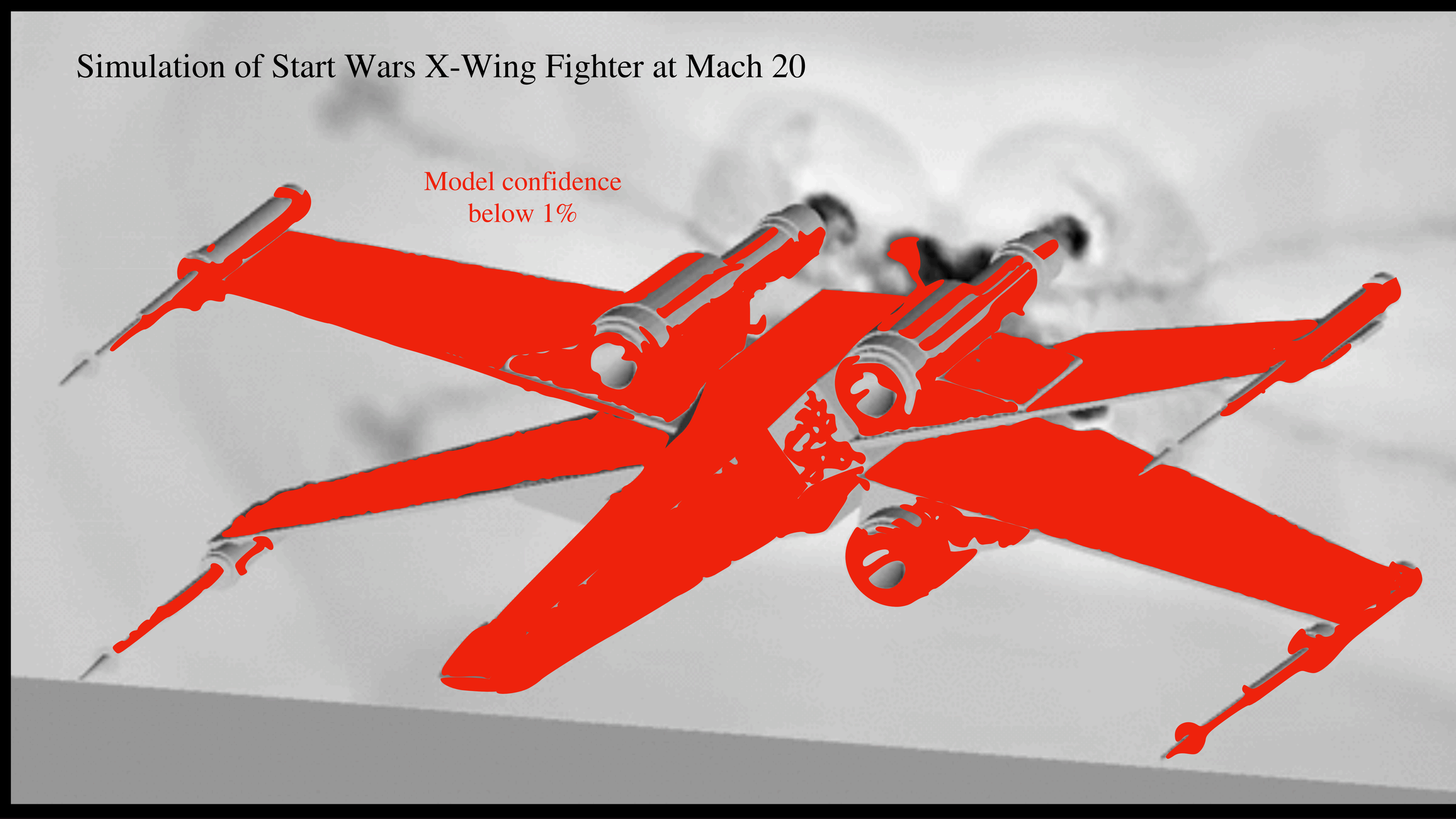
- Consistency between the model and the numerical/gridding schemes is solver-dependent.

- Optimal neural network architecture and reliability, interpretability,…

Simulation of Start Wars X-Wing Fighter at Mach 20



Simulation of Start Wars X-Wing Fighter at Mach 20



Conclusions

- SGS/wall model based on building-block flows

- Main modeling assumption:
  - The building blocks contain the essential flow physics

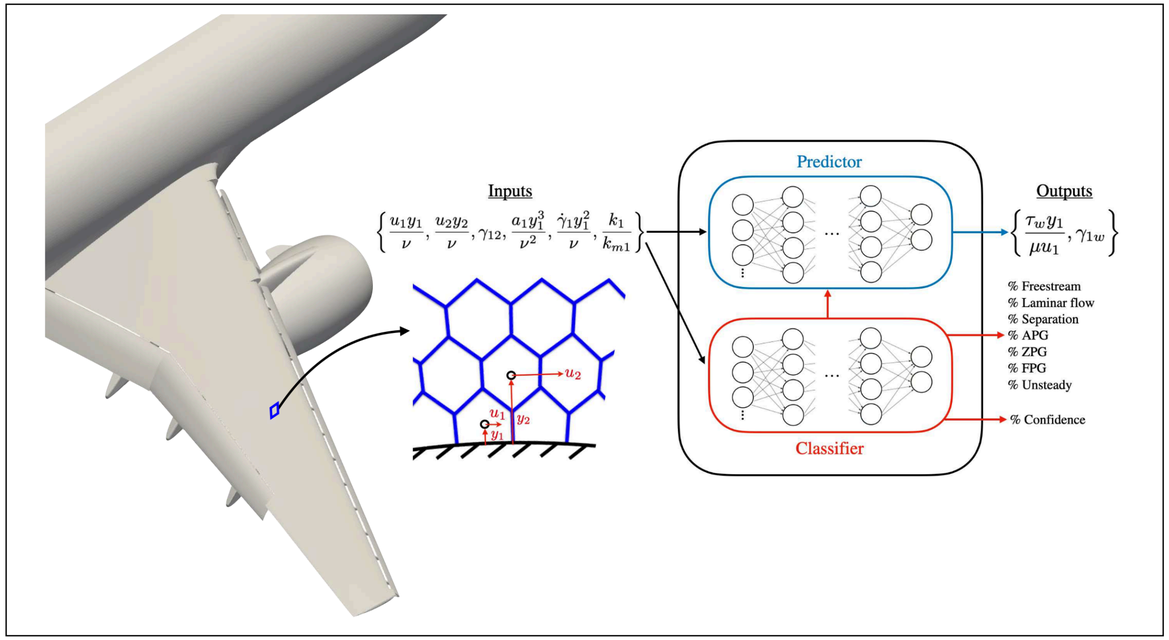
- Building blocks:
  - turbulent channel, adverse/favorable/separated flows, laminar flow,…

- Scalable to more building blocks

- The model comprises two components: classifier + predictor

- Prediction are accompanied by a confidence score

- Improved predictions compared to traditional models in aircraft-like configuration



Lozano-Duran & Bae “Self-critical machine-learning wall-modeled LES for external aerodynamics”, CTR Annual Research Briefs, 2020

Lozano-Duran & Bae “Building-block-flow wall-model for large-eddy simulation”, 2022