USING MACHINE LEARNING FOR WALL FUNCTIONS INCLUDING PRESSURE GRADIENTS

Lars Davidson

LESisMORE, Kickoff, Sept 2024 Download paper and Python scripts

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- In my case, input and output are numerical values.
- The ML will then be some form of regression method.

INITIAL WORK [6]

- Machine Learning (Neural Network) wall functions were developed
- Good results for channel flow placing the wall-adjacent cell at different locations
- Good results for developing boundary layer flow
- Training the Neural Network with steady or instantaneous data: same results
- Training nearest neighbor (Python's scipy.spatial.KDTree) with instantaneous data: same results

- **KDTree** will be used for finding y^+ .
- It is essentially a fast look-up table
- There will be two sets of data points.
 - One is the target data set, i.e. low-Re IDDES ($\mathbf{X} = [U_{target}^+, y_{target}^+]$)
 - The other one is the wall-function IDDES ($\mathbf{x} = [U_{CFD}^+, y_{CFD}^+]$
- KDTree computes the distance between the vectors as

$$\mathbf{d_s} = \mathbf{X}_i - \mathbf{x}_j \tag{1}$$

for all samples i and j and finds the k nearest neighbors for each j.

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- For k and ε , hybrid central/upwind scheme

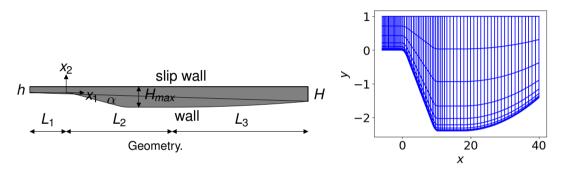
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- cupy is used to switch from CPU to GPU (import cupy)

CREATE TARGET DATABASE 1: DIFFUSER

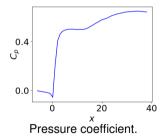


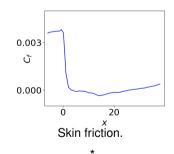
Grid, x - y plane (not to scale). 700×90 cells. Every 10^{th} grid line is shown.

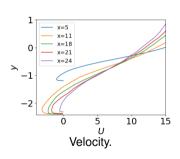
Diffuser, $\alpha = 15^{\circ}$.

TARGET DATABASE: RESULTS

- 700 \times 90 \times 96. $k \varepsilon$ IDDES.
- Inlet b.c. from pre-cursor IDDES channel flow at $Re_{\tau}=5\,200$.

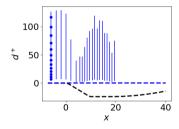




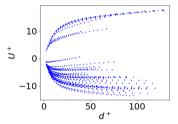


Diffuser flow. Target data base.

Target Database for **KDTree** . Baseline: K = 5 (five NBRS)



Data points of y^+ vs. x.



Scatter plot of U^+ and y^+ .

8/35

Diffuser flow. The target database consists of time-averaged 41 profiles of U^+ vs. y^+ with 26 points in each profile. d the is wall distance. Every second x line and y point are shown.

INPUT/OUTPUT IN THE KDTREE.

 y_P^+ : inlet and outlet parameter U^+ : inlet and output parameter

 u_{τ} : $y_P^+ \nu / y_P$

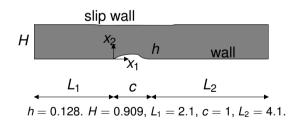
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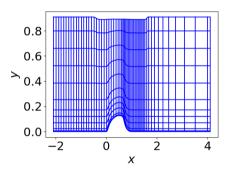
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 u_{τ} : $y_P^+ \nu / y_P$

 $\begin{array}{ccc} \rho u_{\tau}^2 & : & \bar{u} \text{ equation} \\ C_{\mu}^{-1/2} u_{\tau}^2 & : & k \text{ equation} \\ \frac{u_{\tau}^3}{\kappa y} & : & \varepsilon \text{ equation} \end{array}$

CREATE TARGET DATABASE 2: HUMP

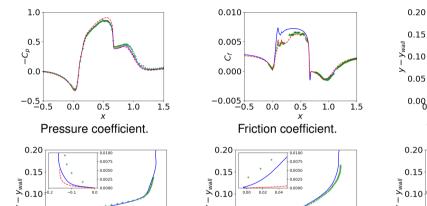




Grid. $582 \times 128 \times 64$ cells. Every 10^{th} .

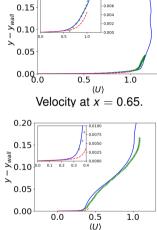
Hump flow.

TARGET DATABASE 2: RESULTS



0.05

0.00



Velocity at x = 1.30.

Velocity at x = 1.10. Hump flow, low-Re IDDES.+: experiments [8, 7].

0.5

 $\langle U \rangle$

1.0

0.02

0.0

0.0

0.5

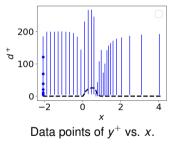
Velocity at x = 0.80.

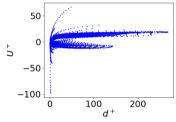
1.0

0.05

0.00

Target Database for **KDTree** . Baseline: K = 1 (one nbr).





Scatter plot of U^+ and y^+ .

Hump flow. d is the wall distance. The target database consists of time-averaged 582 profiles (all grid lines) of U^+ vs. y^+ with 24 points in each profile. Every 20^{th} x line and every 4^{th} y point are shown.

NEW WALL FUNCTION GRID STRATEGY



Low-Re number grid.



Wall function grid.

Different grids. — : grid lines.



New wall function grid.

DIFFUSER FLOW, WALL FUNCTIONS: SETUP

- Wall functions based on KDTree or Reichardt wall functions
- Wall functions based Reichardt's law

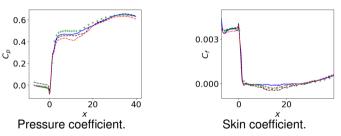
$$rac{ar{u}_P}{u_ au} \equiv U^+ = rac{1}{\kappa} \ln(1 - 0.4y^+) + 7.8 \left[1 - \exp\left(-y^+/11
ight) - \left(y^+/11
ight) \exp\left(-y^+/3
ight)
ight]$$

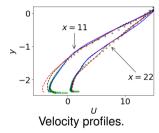
is solved using the Newton-Raphson method scipy.optimize.newton in Python.

- Turbulence model: IDDES based on the AKN low-Re $k \varepsilon$ model
- Instantaneous inlet b.c. from pre-cursor channel IDDES using KDTree wall functions
- Grid: $462 \times 70 \times 48$ (low-Re IDDES grid: $600 \times 90 \times 96$)

Results, Diffuser Flow, $\alpha = 15^{\circ}$

• $468 \times 70 \times 48$ cells (every 2^{nd} in x and z)

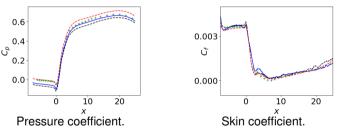


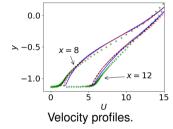


Diffuser flow, $\alpha = 15^o$. — : **KDTree** using hump flow data; ---: **KDTree** using diffuser flow data; ---: Reichardt's law; +: low-Re IDDES.

Results, Diffuser Flow, $\alpha = 10^{\circ}$

• $387 \times 70 \times 48$ cells (every 2^{nd} in x and z)



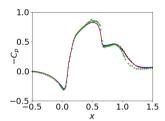


Diffuser flow, $\alpha = 10^o$. — : **KDTree** using hump flow data; ---: **KDTree** using diffuser flow data; ---: Reichardt's law; +: low-Re IDDES.

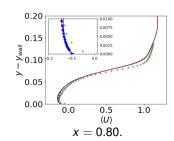
HUMP FLOW, WALL FUNCTIONS: SETUP

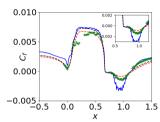
- The Reynolds number is $Re_c = 936\,000$. Spanwise extent is $z_{max} = 0.2$.
- The mesh has $291 \times 106 \times 64/32$ cells [x, y, z] (low-Re IDDES $582 \times 106 \times 64$)
- Inlet b.c.
 - Mean from 2D RANS
 - Inlet turbulence: fluctuation from STG
 - Inlet k and ε : 2D RANS plus commutation term in k eq. [3, 1] (Model 3)
- Comparison with
 - Experiments [8, 7]

Results, Hump Flow. $583 \times 106 \times 64$ Cells.

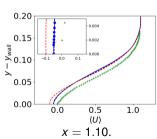


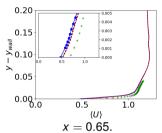
Pressure coefficient.

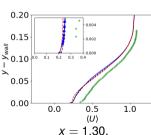




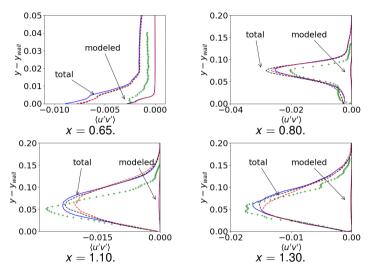
Friction coefficient.



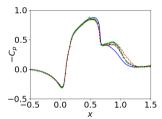




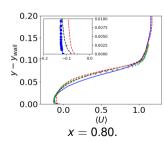
Results, Hump flow. $583 \times 106 \times 64$ cells. Shear Stresses

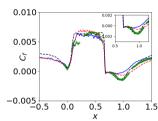


Results, Hump Flow. 291 \times 106 \times 32 Cells.

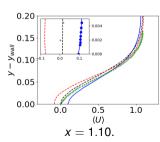


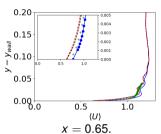
Pressure coefficient.

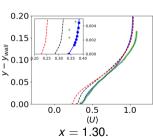




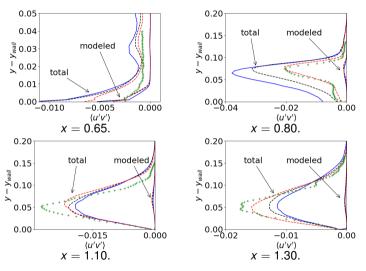
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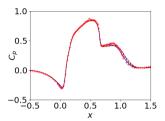




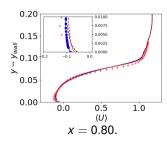
Results, Hump flow. $291 \times 106 \times 32$ cells. Shear Stresses

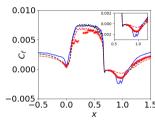


Results, Hump Flow. 291 \times 106 \times 32 Cells, K = 5.

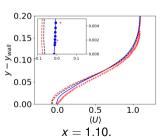


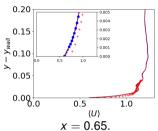
Pressure coefficient.

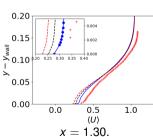




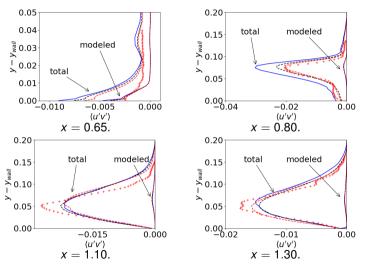
Friction coefficient.





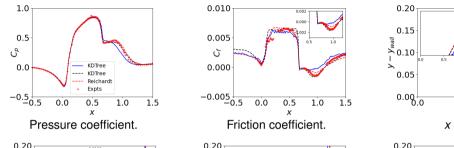


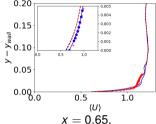
Hump flow. 291 \times 106 \times 32 cells. Shear Stresses, K=5.

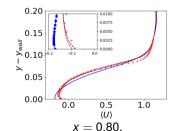


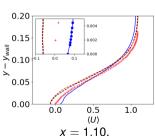
- : KDTree hump data; - - - : KDTree diffuser data; - - : Reichardt's law; +: exp.

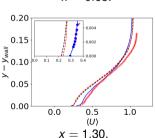
RESULTS, HUMP FLOW. $291 \times 106 \times 16$ CELLS. VELOCITY





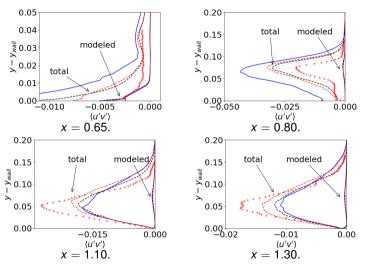






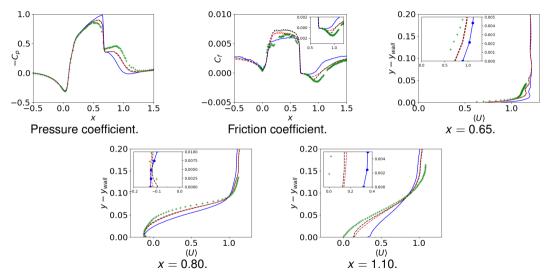
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Results, Hump Flow. 291 \times 106 \times 16 cells. Shear Stresses



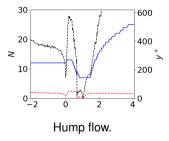
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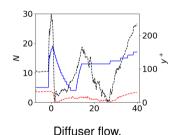
Results, Hump Flow. Standard Wall Function Mesh, $N_v = 80$



-: KDTree hump data; ---: KDTree diffuser data; --: Reichardt's law; +: exp.

URANS/LES INTERFACE.



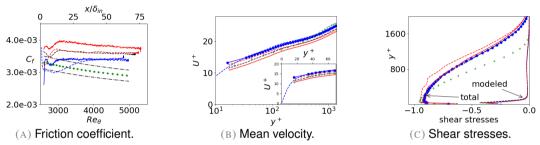


— : Number of cells in the URANS region (left y axis); — — : y^+ of wall-adjacent cells (right y axis).

BOUNDARY LAYER FLOW.

- Inlet b.c. taken from a pre-cursor $k-\omega$ simulation at $Re_{\theta} \simeq 2500$
- Grid: $550 \times 90 \times 64$
- Domain: $63 \times 4.6 \times 3.2$.
- Inlet boundary layer thickness: $\delta_{in} = 0.86$
- Inlet k and ε : 2D RANS plus commutation term in k eq. [4, 1].
- Synthetic fluctuations [12, 2] are superimposed on the mean flow

BOUNDARY LAYER FLOW. RESULTS. 3rd CELL.

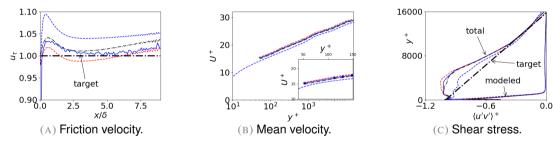


 u_{τ} is computed by using U^+ and y^+ at the 4th cell. Velocity and shear stresses are shown at $Re_{\theta}=4\,000$. —: **KDTree**, hump flow ---: **KDTree**, diffuser flow data, K=5; —: **KDTree**, diffuser flow data, K=1; —-: Reichardt's wall function; •: cell centers; —-: low-Re IDDES; *: $C_f=2(1/0.384\ln(Re_{\theta})+4.127)^{-2}$; —-: $\pm 6\%$; +: DNS.

CHANNEL FLOW.

- $Re_{\tau} = 16\,000$, Inlet-outlet
- Grid: $96 \times 32 \times 32$
- Domain: $9 \times 2 \times 1.6$
- Inlet k and ε : 2D RANS plus commutation term in k eq. [4, 1].
- Synthetic fluctuations [12, 2] are superimposed on the mean flow

CHANNEL FLOW. RESULTS.



Velocity and shear stress are shown at $x/\delta=6$. — : **KDTree** , hump flow _ - - : **KDTree** , diffuser flow; — - : low-Re IDDES; — : **KDTree** , hump flow , K=5; — - : Reichardt's wall function; •: cell centers: +: Reichardt's law

CONCLUSIONS

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- Much more target data (many more x profiles) are needed in the hump flow than in the diffuser flow
- You can downlload Python scripts here

- [1] S. Arvidson, L. Davidson, and S.-H. Peng. Interface methods for grey-area mitigation in turbulence-resolving hybrid RANS-LES. *International Journal of Heat and Fluid Flow*, 73:236–257, 2018.
- [2] M. Carlsson, L. Davidson, S.-H. Peng, and S. Arvidson. Investigation of turbulence injection methods in large eddy simulation using a compressible flow solver. In *AIAA Science and Technology Forum and Exposition, AIAA SciTech Forum*, 2022.
- [3] L. Davidson. Zonal PANS: evaluation of different treatments of the RANS-LES interface. *Journal of Turbulence*, 17(3):274–307, 2016.
- [4] L. Davidson. Two-equation hybrid RANS-LES models: A novel way to treat k and ω at inlets and at embedded interfaces. *Journal of Turbulence*, 18(4):291–315, 2017.
- [5] L. Davidson. pyCALC-LES: a Python code for DNS, LES and Hybrid LES-RANS. Division of Fluid Dynamics, Dept. of Mechanics and Maritime Sciences, Chalmers University of Technology, Gothenburg, 2021.

- [6] L. Davidson. Using machine learning for formulating new wall functions for Detached Eddy Simulation. In 14th International ERCOFTAC Symposium on Engineering Turbulence Modelling and Measurements (ETMM14), Barcelona/Digital, Spain 6–8 September, 2023.
- [7] D. Greenblatt, K. B. Paschal, C.-S. Yao, and J. Harris. A separation control CFD validation test case Part 1: Zero efflux oscillatory blowing. AIAA-2005-0485, 2005.
- [8] D. Greenblatt, K. B. Paschal, C.-S. Yao, J. Harris, N. W. Schaeffler, and A. E. Washburn. A separation control CFD validation test case. Part 1: Baseline & steady suction. AIAA-2004-2220, 2004.
- [9] Andreas Lindholm, Niklas Wahlström, Fredrik Lindsten, and Thomas Schön. *Machine Learning: A First Course for Engineers and Scientists*. Cambridge University Press, 2022.

- [10] Menneni Rachana, Jegadeesan Ramalingam, Gajula Ramana, Adigoppula Tejaswi, Sagar Mamidala, and G Srikanth. Fraud detection of credit card using machine learning. *GIS-Zeitschrift für Geoinformatik*, 8:1421–1436, 10 2021.
- [11] Sudarshana S Rao and Santosh R Desai. Machine learning based traffic light detection and ir sensor based proximity sensing for autonomous cars. In *Proceedings of the International Conference on IoT Based Control Networks & Intelligent Systems ICICNIS*, 2021.
- [12] M. Shur, P.R. Spalart, M.K. Strelets, and A.K. Travin. Synthetic turbulence generators for RANS-LES interfaces in zonal simulations of aerodynamic and aeroacoustic problems. *Flow, Turbulence and Combustion*, 93:69–92, 2014.