Advanced Modeling & Simulation (AMS) Seminar Series
NASA Ames Research Center, May 8th, 2025

Near-Wall Modeling for Rough-Wall Turbulent Boundary Layer Flows with Heat Transfer

Xiang Yang
xzy48@psu.edu

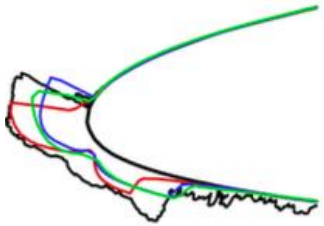
PennState

supercooled water droplets in clouds hit the aircraft and freeze upon contact

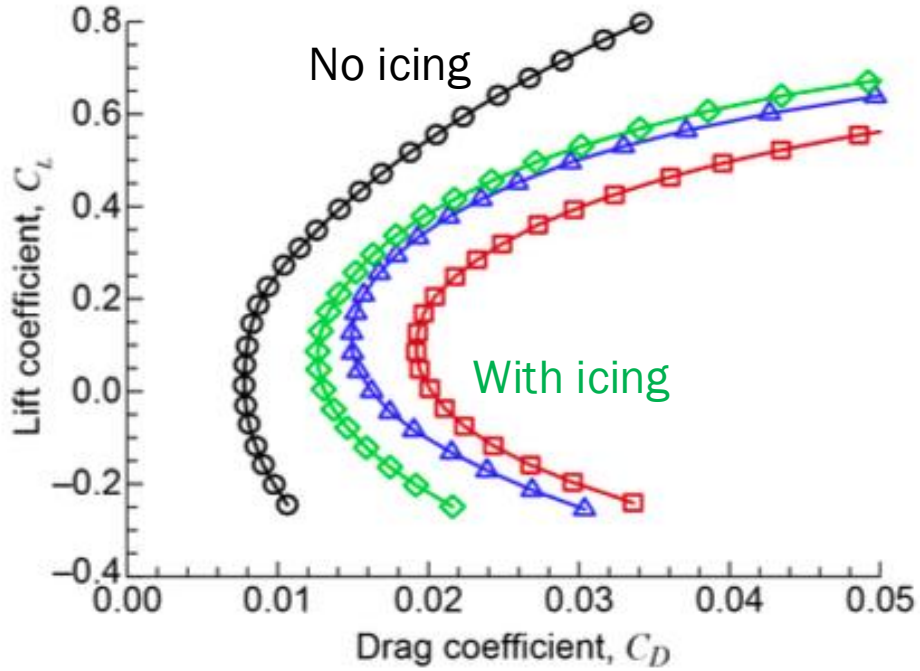
Motivation: Icing

Ice build up →



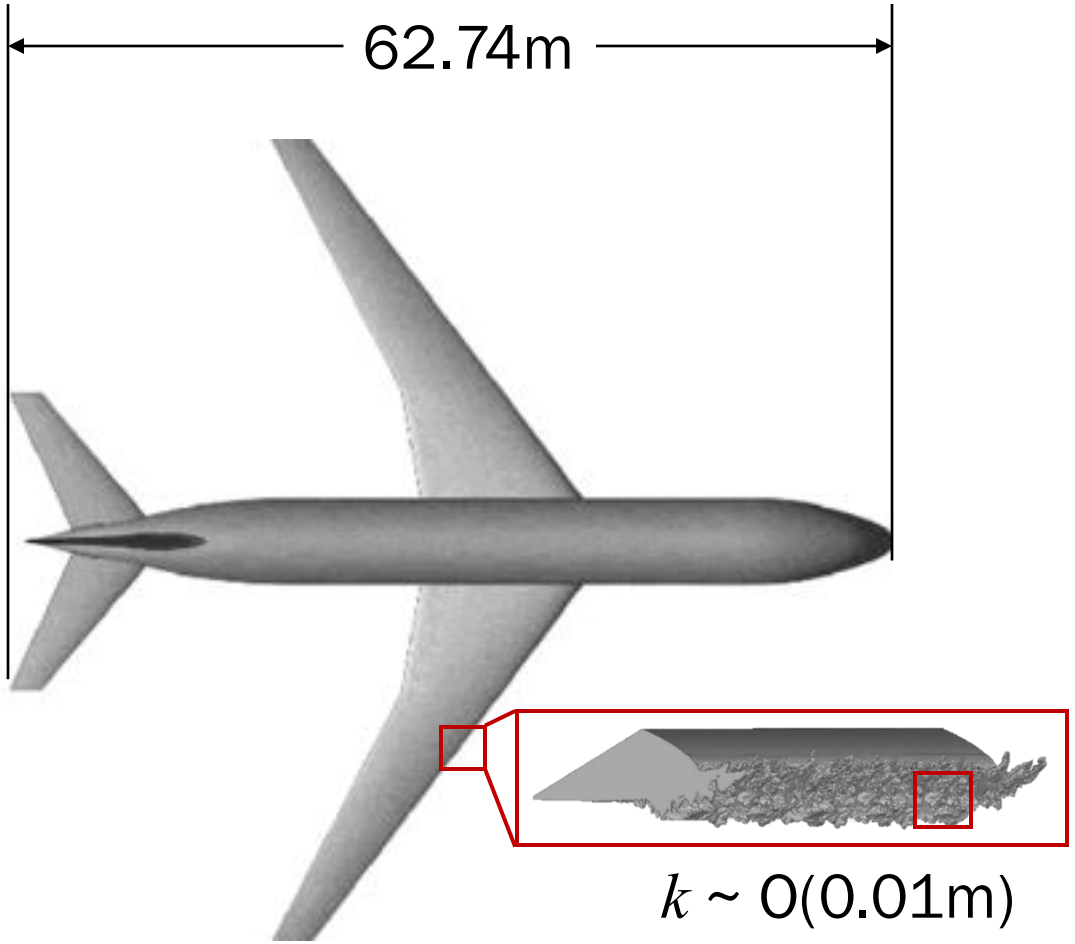


Reduced lift, increased drag



Broeren, A., Lee, S., Bragg, M., Woodard, B., Radenac, E., & Moens, F. (2022). (NASA/TP-20210023843).

Motivation: Predictive Modeling is Challenging



NASA CRM

scale separation → high cost

-Craig Penner, D., Sousa, V., Ravikumar, K., Saurabh, K., Cadieux, F., Stich, G. D., ... & Duensing, J. C. (2025). In *AIAA SCITECH Forum* (p. 0059).
-Bornhoft, B. J., Jain, S. S., Bose, S. T., & Moin, P. (2024). In *AIAA SCITECH Forum* (p. 1336).

Challenge: the challenge is not unique to icing

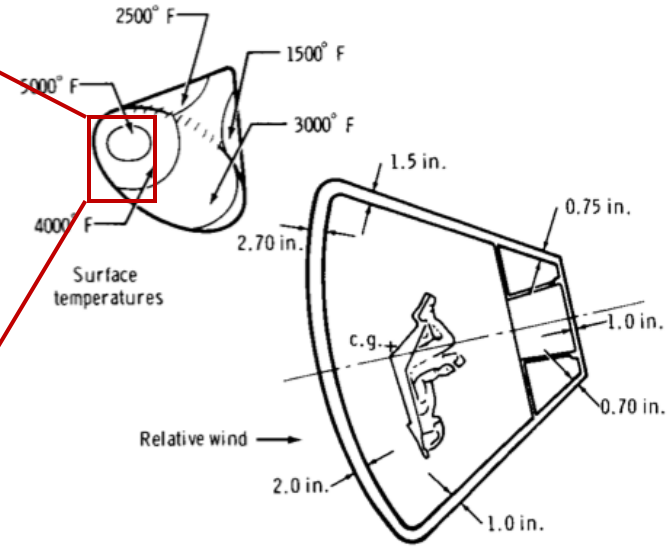




k ~ O(10 mm)

Aircraft Engine: thermal degradation, oxidation, coating erosion.

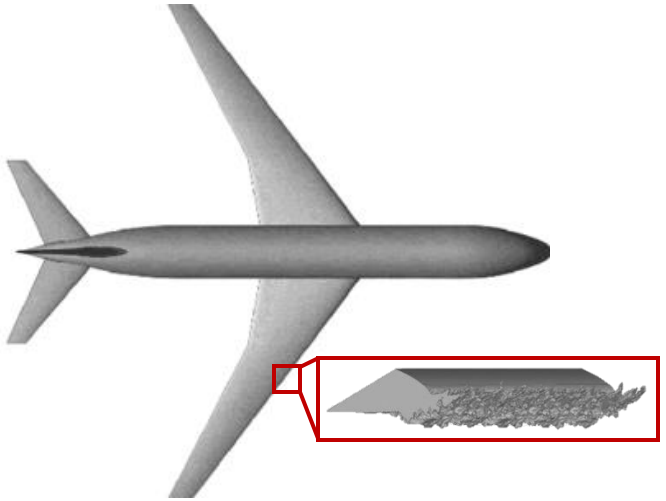




Reentry vehicle: ablation, material manufacturing imperfection.

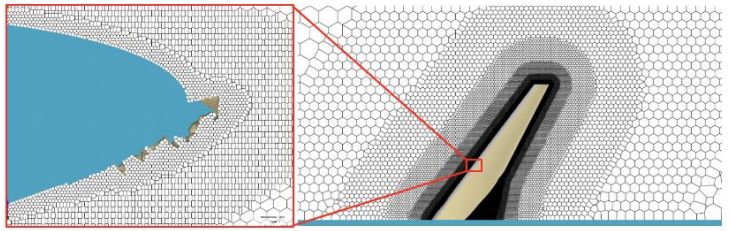
Motivation: Top-Down Solution

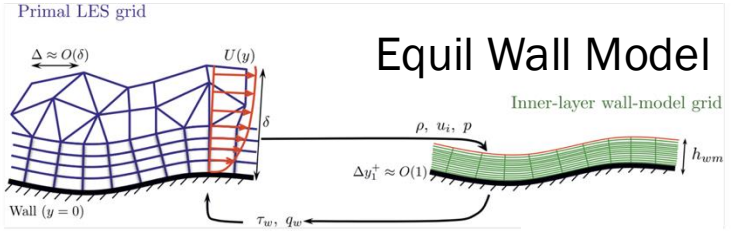
Full geometry →



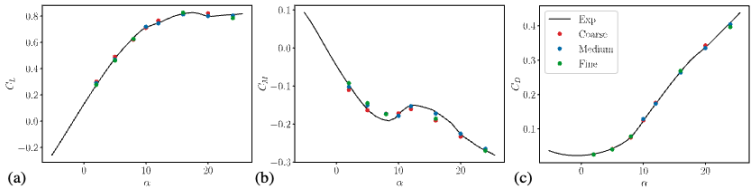
Computational tools →

Voronoi Grid





Solution



Lift Moment Drag

-- No need for model development

-- Costly [in terms of computational hours]

Motivation: Bottom-Up Solution

Model development

Motivation

-- EWM: accounts for unresolved constant stress layer

-- Missing physics

-- Missing best practices

- Constrained by development cycle

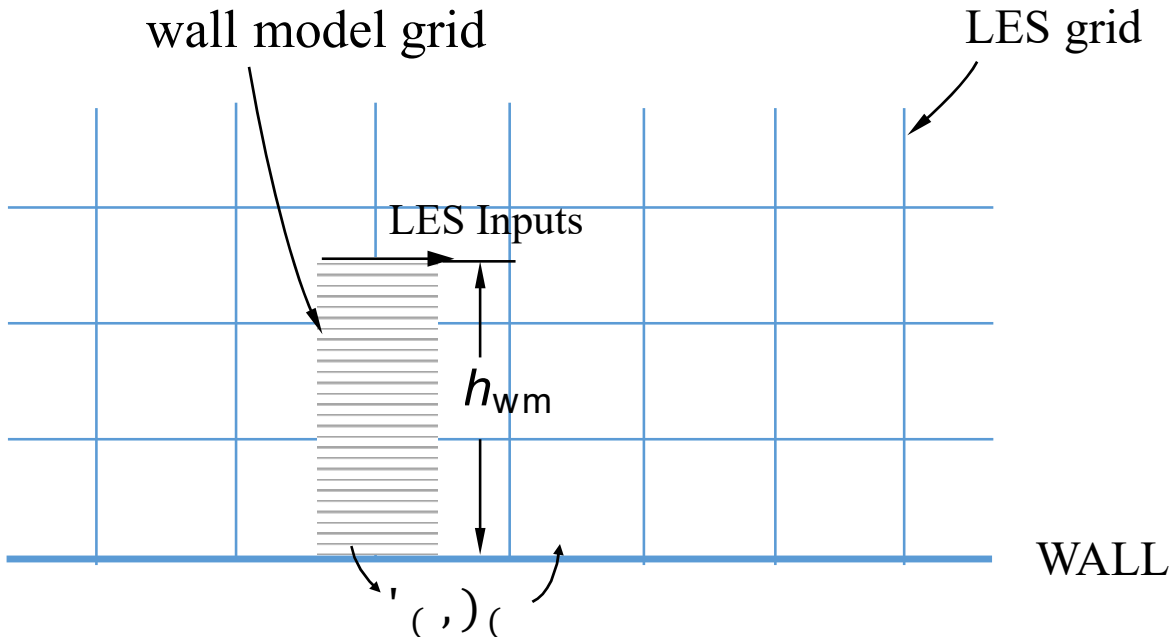
This Talk

EWM and its immediate extensions

- Surface roughness: partly resolved/unresolved surface roughness
- Heat transfer: smooth wall
- Heat transfer: fully resolved surface roughness
- Heat transfer: partly resolved surface roughness
- Pressure gradient

--We will focus on simple geometries, involving new physics one at a time.
--Numerics: 2nd order discretization in space, 2nd/3rd order discretization in time.
--Typical grid resolution for WMLES of channel O(10-30) grid points per half channel height.

Equil WM Setup



Imposes the LoW instantaneously and locally $\tau_w/\rho = \left[\frac{U_{\mathrm{LES}}}{\mathrm{LoW}(h^+_{\mathrm{wm}})}\right]^2$.

LoW reduces to $U^+ = \frac{1}{\kappa}\ln(y^+) + B$ in the logarithmic layer.

We will get to ODE-based model..

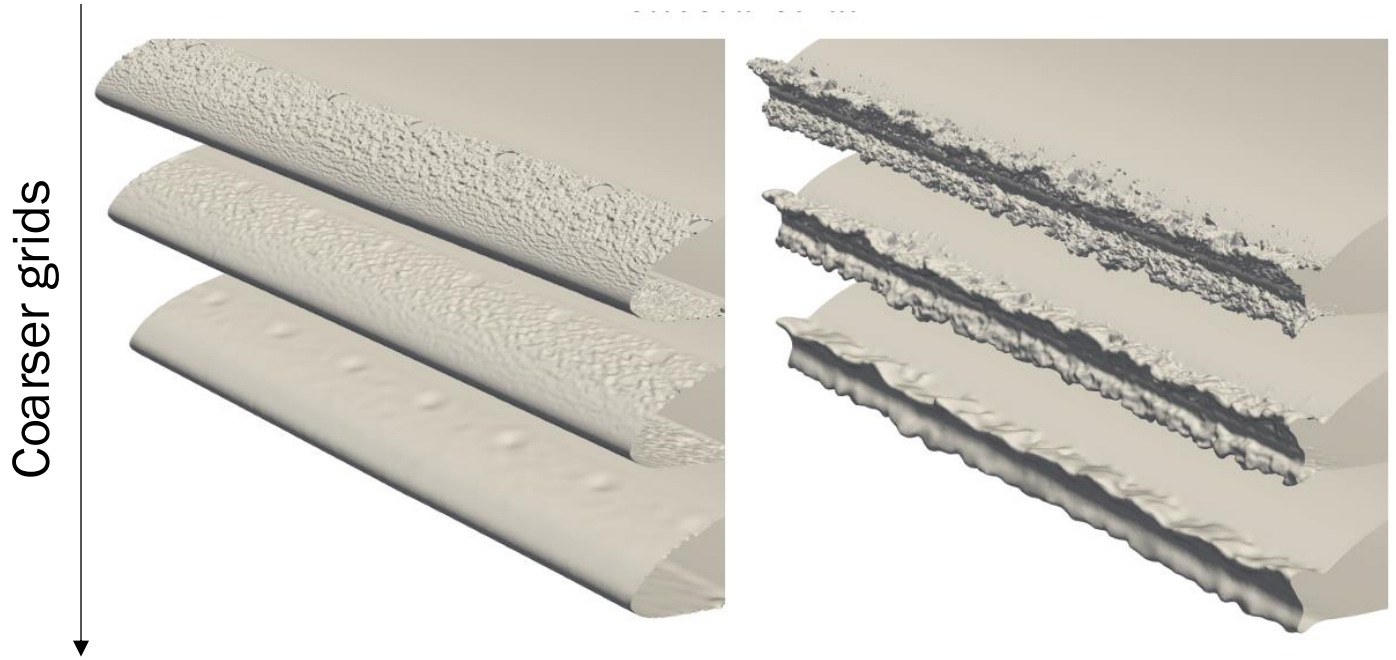
Outline of the Talk

EWM and its immediate extensions

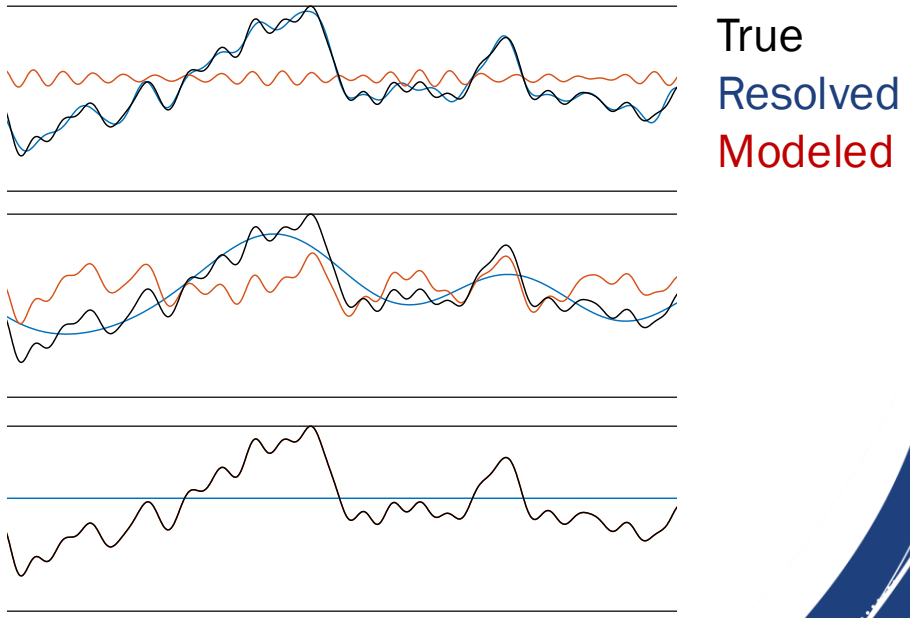
- Surface roughness: partly resolved/unresolved surface roughness
- Heat transfer: smooth wall
- Heat transfer: fully resolved surface roughness
- Heat transfer: partly resolved surface roughness
- Pressure gradient

Flow Problem: Roughness is partly resolved

Icing on Airfoil

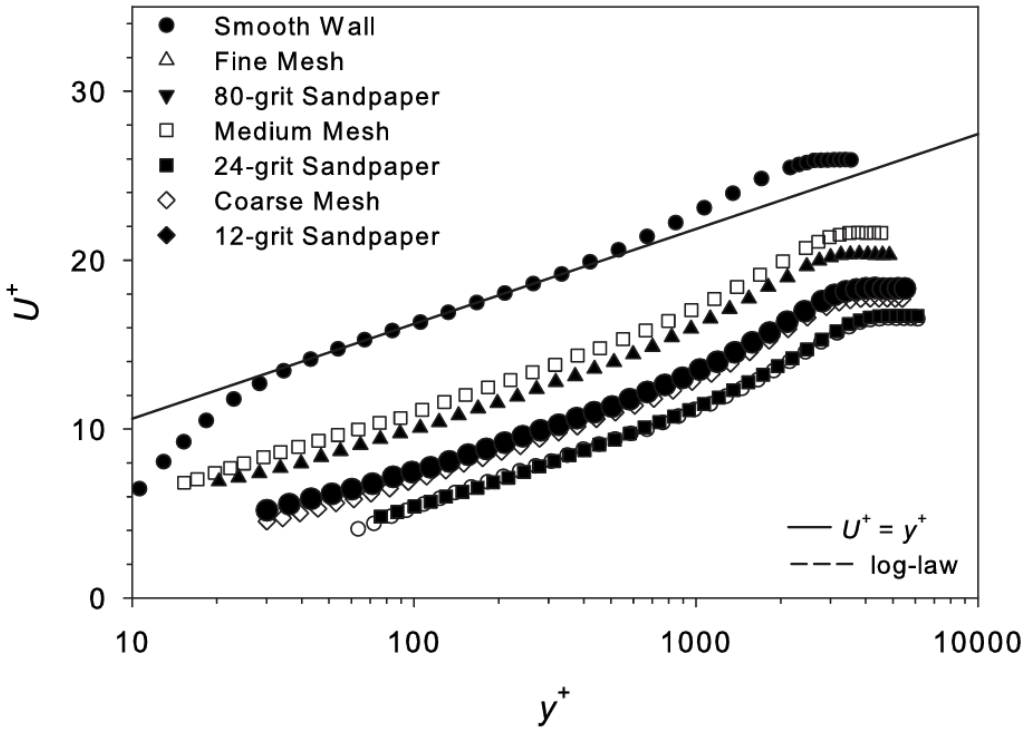


General surface roughness



Bellosta, T., Donizetti, A., Zabaleta, F., Bornhoft, B., Jain, S., Bose, S., & Guardone, A. (2024). *CTR Summer Program Proceedings*, 24, 427–435.

Flow Physics: Rough Law of the Wall



Flack, K. A., & Schultz, M. P. (2010). *Journal of Fluids Engineering*, 132(4), 041203.

-- The LoW

$$U^+ = \frac{1}{\kappa}\ln(y^+) + B - \Delta U^+$$

Roughness function

-- Also

$$U^+ = \kappa^{-1}\ln\left[(y-d)/k_s\right] + A$$

Roughness morphology → $\Delta U^+, k_s$?

Roughness Model: Empirical Models

Empirical correlations

$$k_s = f(\text{roughness statistics})$$

Examples

Forooghi et al 2017 $k_s/k_z = 1.07(0.67\mathrm{Sk}^2 + 0.93\mathrm{Sk} + 1.3)(1 - e^{-3.5\mathrm{ES}})$

Barros et al 2018 $k_s/k_{\mathrm{rms}} = 3.41(1 + \mathrm{Sk})^{0.61}$

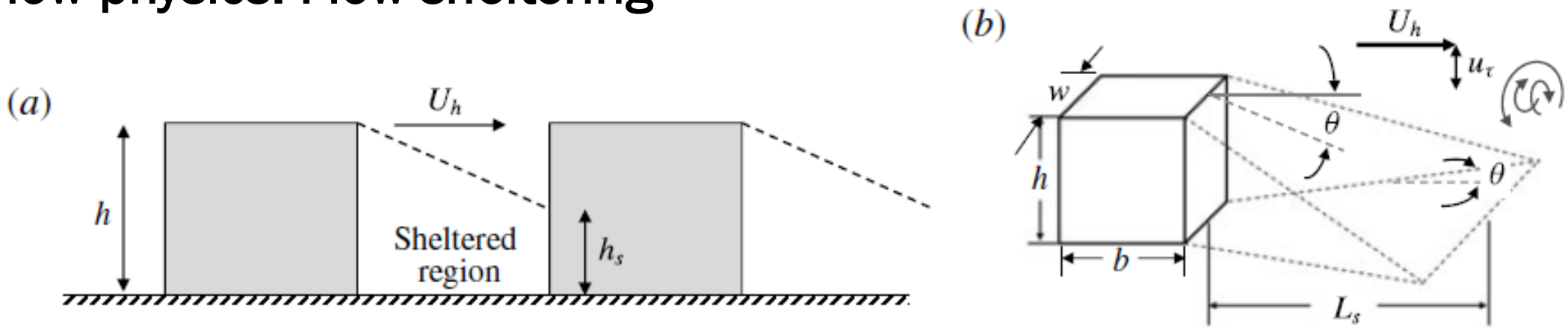
Flack et al 2020

$$k_s/k_{\mathrm{rms}} = \begin{cases} 2.48(1 + \mathrm{Sk})^{2.24} & Sk > 0 \\ 2.11, & Sk = 0 \\ 2.73(1 + \mathrm{Sk})^{-0.45} & Sk < 0 \end{cases}$$

Jouybari et al 2021 f is a neural network

Roughness Model: Physical Models

Flow physics: Flow sheltering

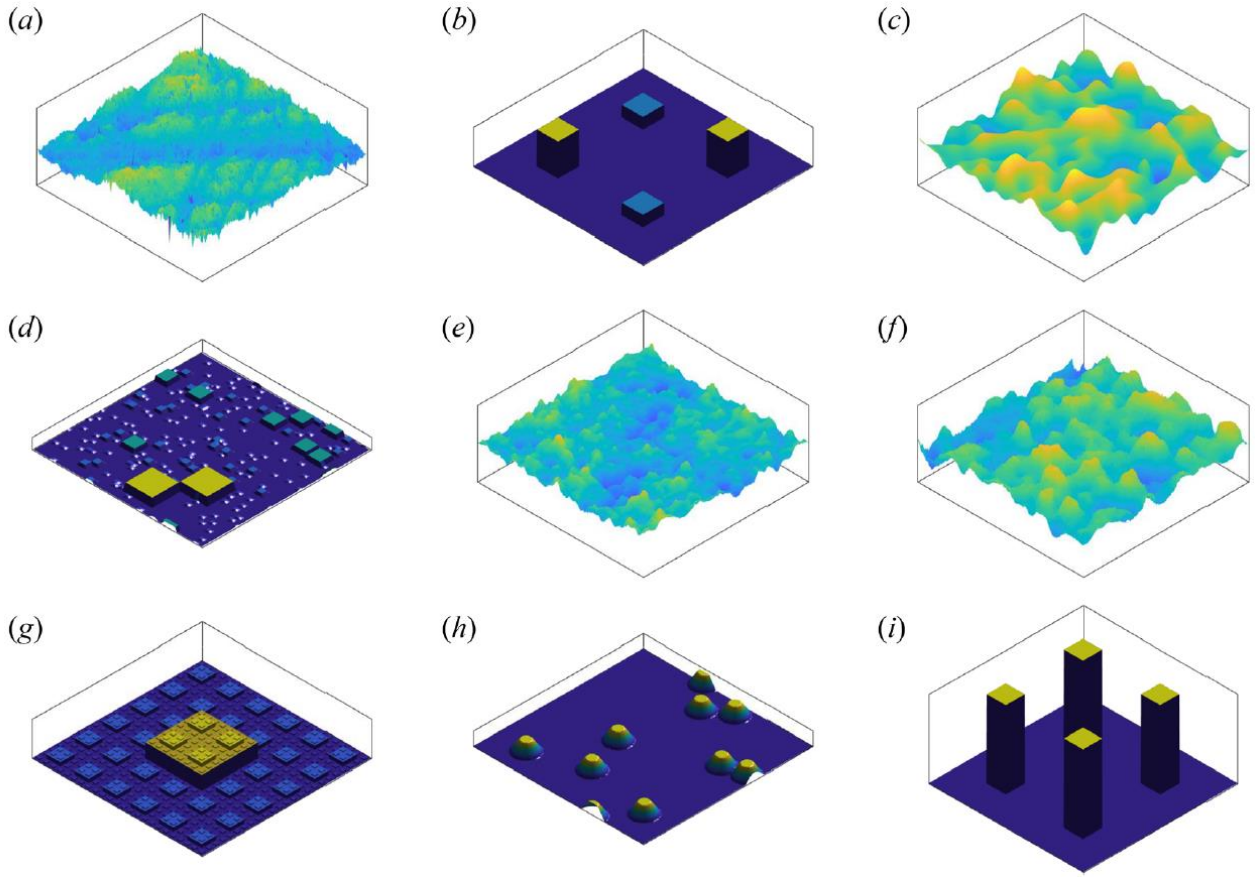


Yang, X., Sadique, J., Mittal, R., & Meneveau, C. (2016). Exponential roughness layer and analytical model for turbulent boundary layer flow over rectangular-prism roughness elements. *Journal of Fluid Mechanics*, *789*, 127-165.

Pick a rough-wall model?

Roughness Database

https://roughnessdatabase.org/

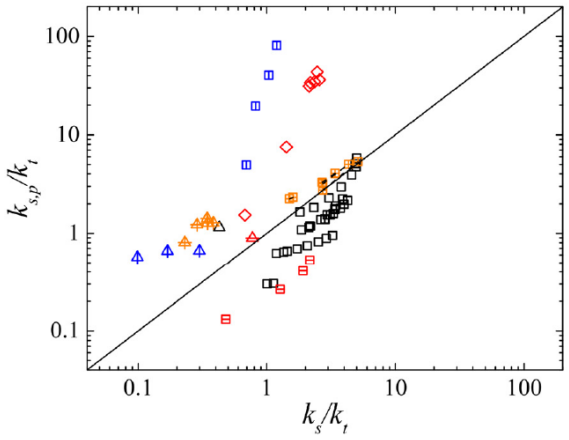


Roughness type	References	Measurement type
Bi-directional sanded	Schultz and Flack [37]	Experiment
Cuboids	Yang et al. [28]	Simulation
Grit-blasted	Thakkar et al. [38]	Simulation
Fractal-like cuboids	Yang and Meneveau [39]	Simulation
Power-law	Barros et al. [24]	Experiment
Gaussian	Flack et al. [23]	Experiment
Multiscale cuboids	Medjnoun et al. [40]	Experiment
Truncated cones	Womack et al. [41]	Experiment
Deep (slender) rectangular	Zhang et al. [31]	Simulation

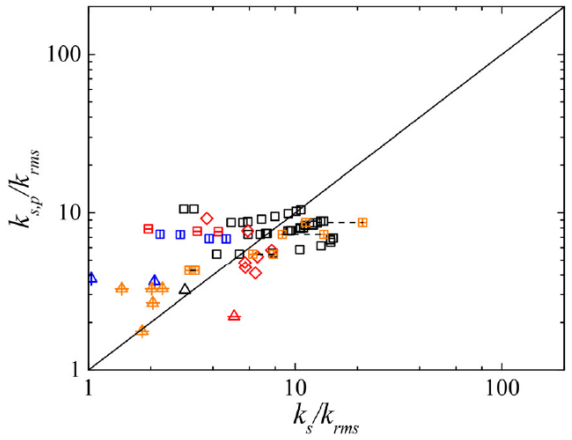
Results of a Survey

Prediction v.s. measurements

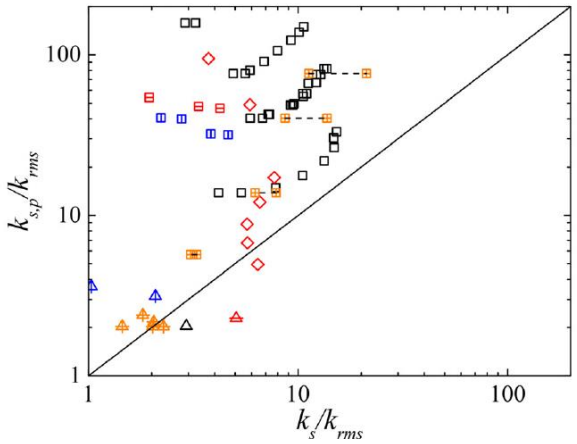
Alg cor: Forooghi et al 2017



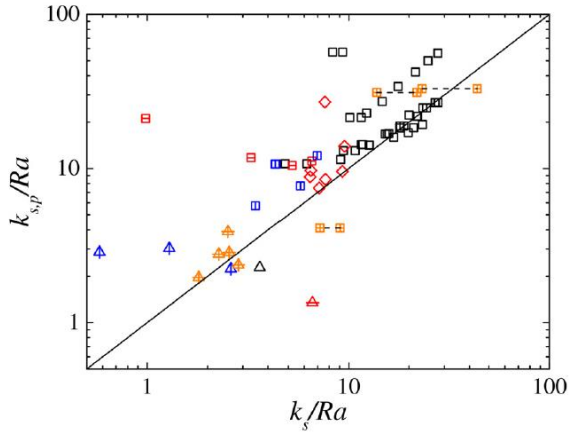
Alg cor: Barros et al 2018



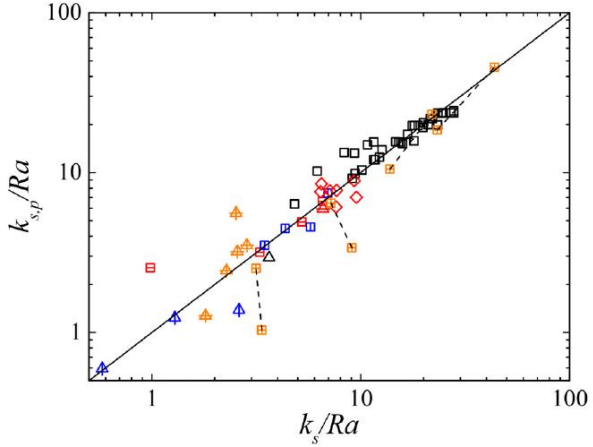
Alg cor: Flack et al 2020



ML: Jouybari et al 2021



Phys: Yang et al. 2016

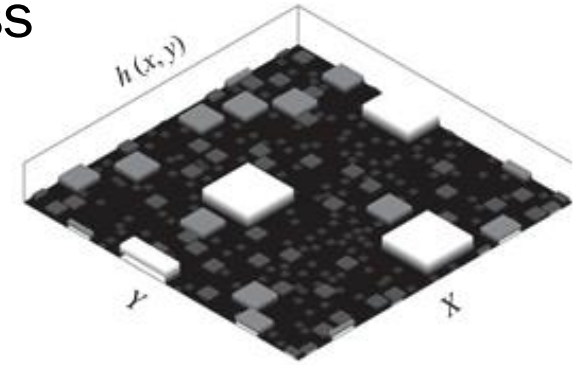


Physics-based flow sheltering model generalizes reasonably well.

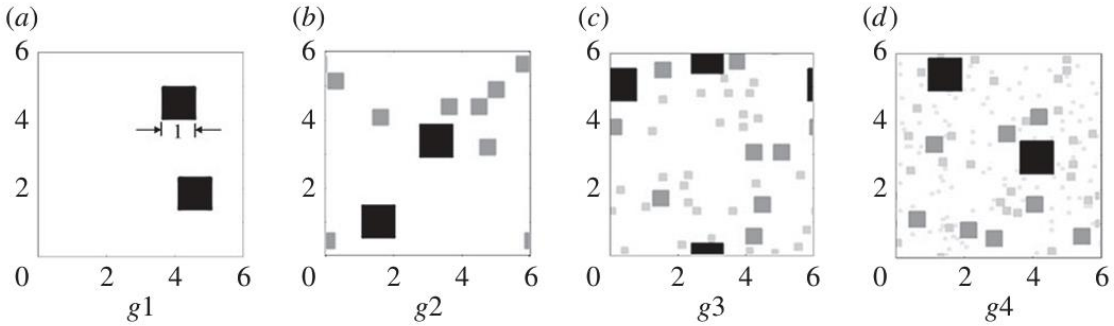
Yang, X., Zhang, W., Yuan, J., & Kunz, R. F. (2023). *Journal of Fluids Engineering*, *145*(10).

A case study

Target Roughness

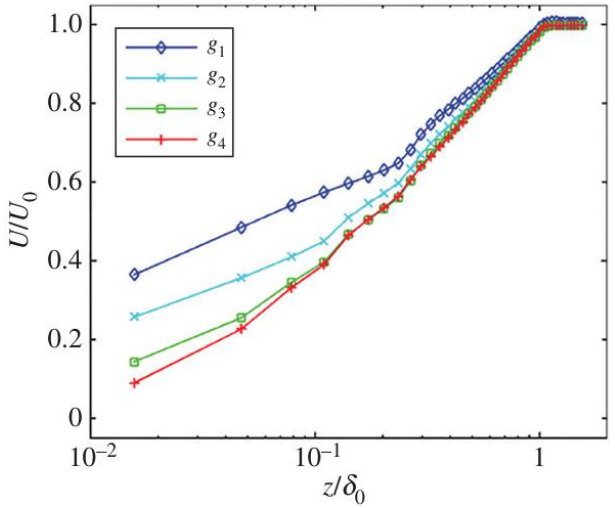


Various levels of resolved roughness

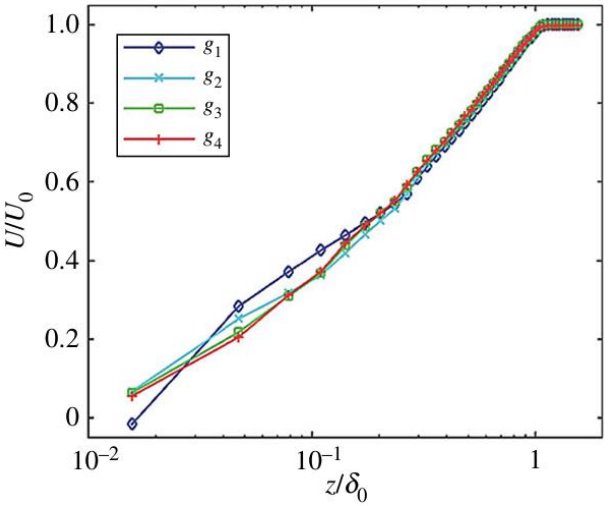


Roughness modeling makes up for unresolved roughness on a coarse grid.

EWM,
Unresolved roughness is not accounted for



Rough EWM,
Unresolved Roughness is accounted for



Yang, & Meneveau, (2017). *Philosophical Transactions of the Royal Society A*, *375*(2091), 20160098.

Take-home Message

- Applying the wall model directly without accounting for unresolved roughness leads to underpredictions of the drag force.
- Rough WM makes up for the unresolved surface roughness, yielding consistent results across a range of grids.

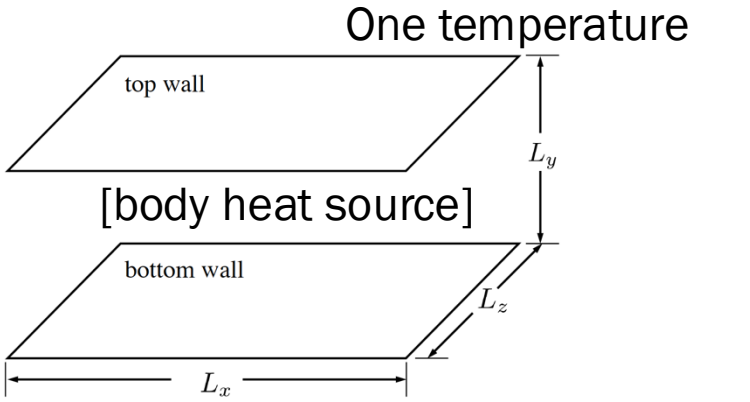
Outline of the Talk

EWM and its immediate extensions

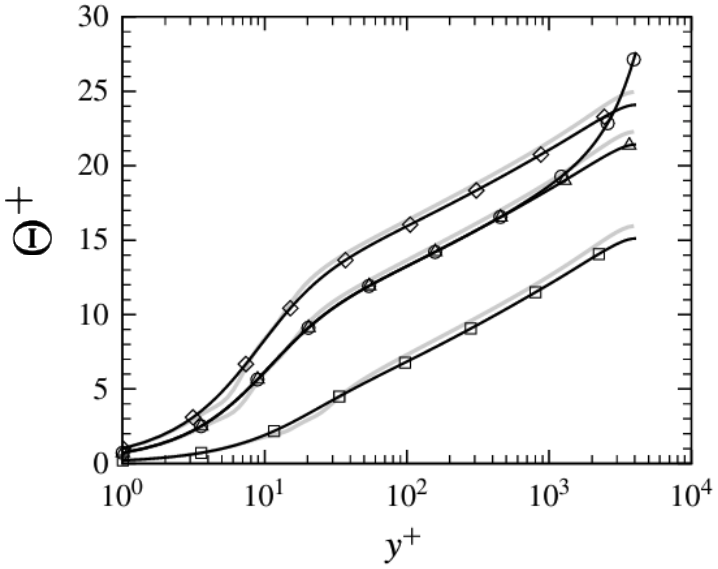
- Surface roughness: partly resolved/unresolved surface roughness
- Heat transfer: smooth wall
- Heat transfer: fully resolved surface roughness
- Heat transfer: partly resolved surface roughness
- Pressure gradient

Heat Transfer

Flow Problem



Mean Temperature



-- LoW

$$\Theta^+ = \frac{1}{\kappa}\ln(y^+) + B(Pr)$$

Pirozzoli, S., Bernardini, M., & Orlandi, P. (2016). *Journal of Fluid Mechanics*, *788*, 614-639.

Near-wall Modeling for Heat Transfer

The LoW-based wall model (algebraic)

$$q_w/\rho = C_p T_\tau u_\tau \qquad u_\tau = \frac{U_{\mathrm{LES}}}{f(h^+_{\mathrm{wm}})} \qquad T_\tau = \frac{\Theta_{\mathrm{LES}}}{f_T(h^+_{\mathrm{wm}})}$$

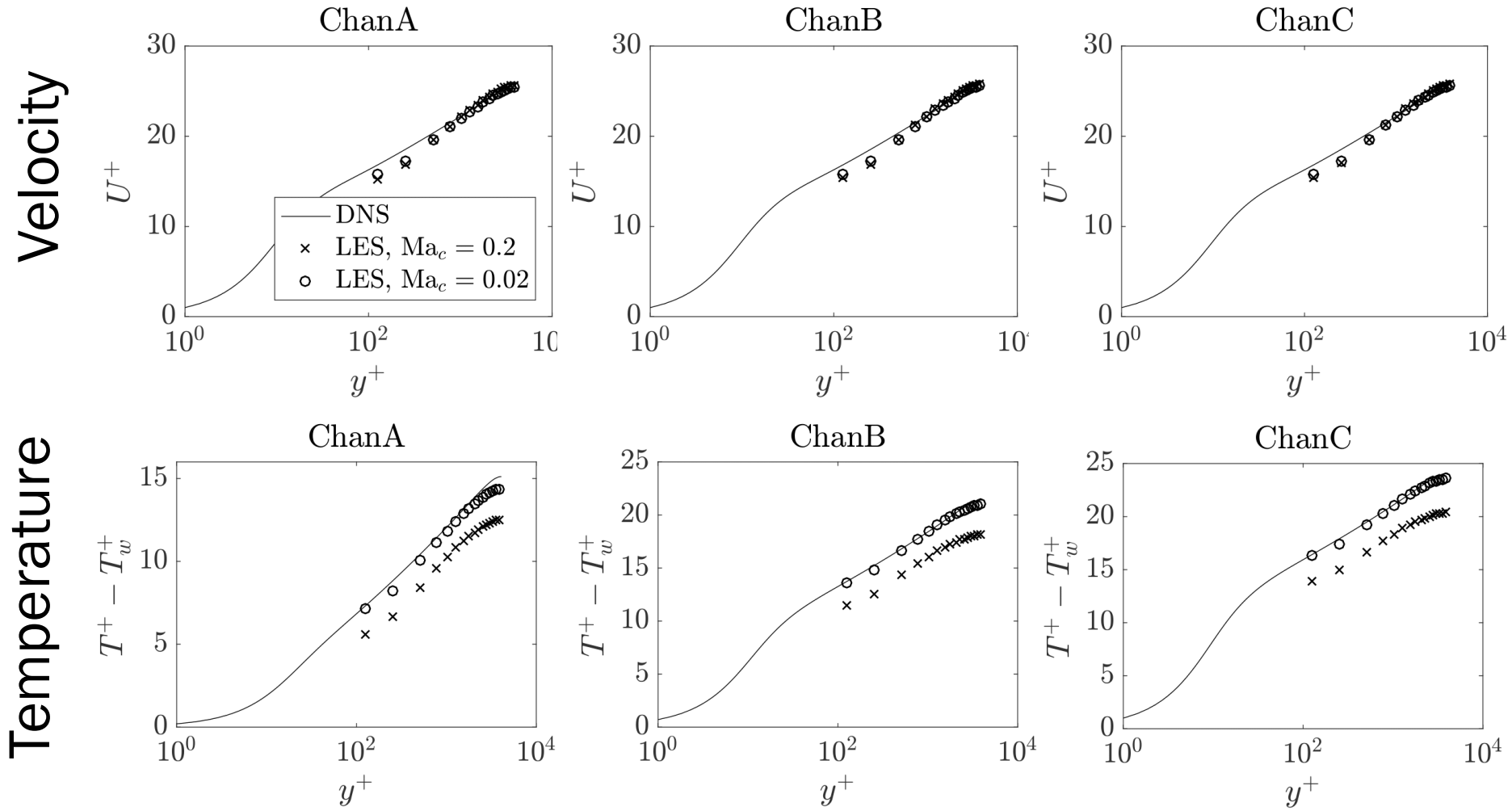
The LoW-based wall model (ODE)

$$\frac{d}{dy}\left[(\mu+\mu_{t,\mathrm{wm}})\frac{dU_\parallel}{dy}\right]=0, \quad \frac{d}{dy}\left[(\mu+\mu_{t,\mathrm{wm}})U_\parallel\frac{dU_\parallel}{dy}+c_p\left(\frac{\mu}{Pr}+\frac{\mu_{t,\mathrm{wm}}}{Pr_{t,\mathrm{wm}}}\right)\frac{dT}{dy}\right]=0,$$

$$\mu_{t,\mathrm{wm}} = \kappa\rho y\sqrt{\frac{\tau_w}{\rho}}\mathcal{D}, \quad \mathcal{D}=[1-\exp(-y^+/A^+)]^2, \ \kappa=0.41, \ Pr_{t,wm}=0.9, \ A^+=17$$

The two models are identical at low speeds.

Channel Flow with Heat Transfer



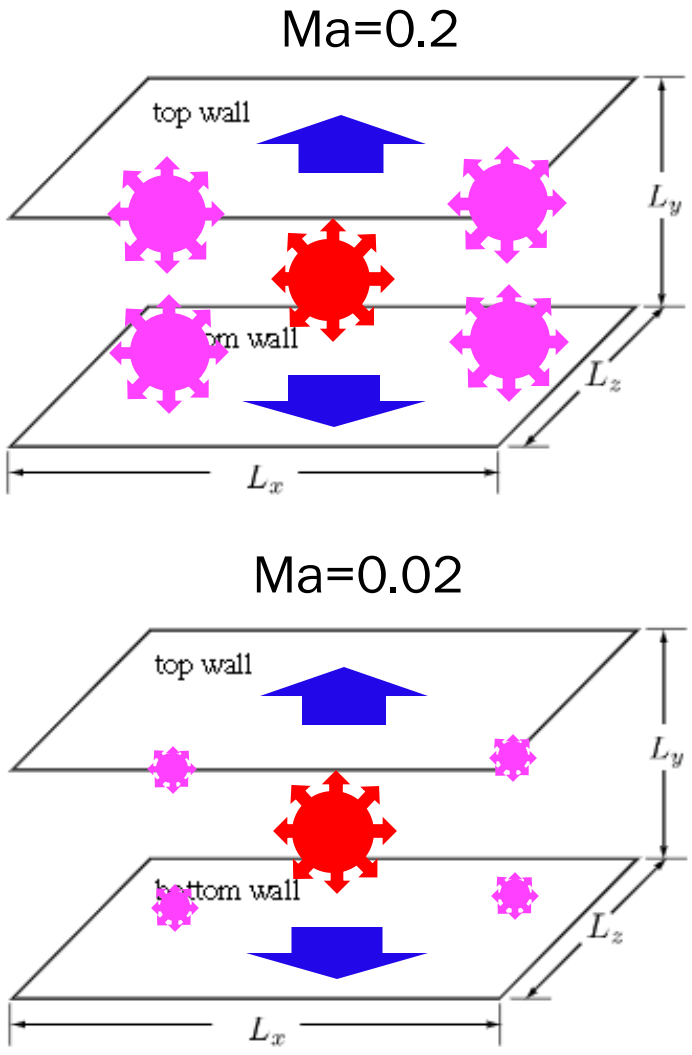
Compressibility effect is almost always non-negligible for heat transfer problems.

Flow Physics

Energy transport equation

$$\rho\frac{De}{Dt} = \underbrace{\nabla\cdot(k\nabla T)}_{\text{Conduction}} - p\nabla\cdot\mathbf{u} + \underbrace{Q}_{\text{Body heating}} + \overbrace{\Phi}^{\text{Viscous heating}}$$

Viscous heating adds to the wall heat flux, leading to a larger T_τ and a smaller T^+.



Xu, H. H., Yang, X. I., & Milani, P. M. (2021). Assessing wall-modeled large-eddy simulation for low-speed flows with heat transfer. *AIAA Journal*, *59*(6), 2060-2069.

Account for Heat Transfer at Finite Mach Number

Baseline Model

$$\frac{d}{dy}\left[(\mu+\mu_{t,\mathrm{wm}})\frac{dU_{\parallel}}{dy}\right]=0,\quad \frac{d}{dy}\left[(\mu+\mu_{t,\mathrm{wm}})U_{\parallel}\frac{dU_{\parallel}}{dy}+c_p\left(\frac{\mu}{Pr}+\frac{\mu_{t,\mathrm{wm}}}{Pr_{t,\mathrm{wm}}}\right)\frac{dT}{dy}\right]=0,$$

$$\mu_{t,\mathrm{wm}}=\kappa\rho y\sqrt{\frac{\tau_w}{\rho}}\mathcal{D},\quad \boxed{\mathcal{D}}=[1-\exp(-y^+/A^+)]^2,\ \kappa=0.41,\ \boxed{Pr_{t,wm}}=0.9,\ A^+=17$$

Improvements

$$\boxed{D}=[1-\exp(-y^*/A^+)]^2\quad \boxed{Pr_{t,\epsilon}}=\frac{\mu_t}{\alpha_t}=\frac{\kappa}{\kappa_T}\frac{[1-\exp(-y^*/A)]^2+A_T\epsilon}{[1-\exp(-y^*/A_T)]^2+A\epsilon}$$

Yang & Lv, *Theor Comput Fluid Dyn,* 2018, 1-11

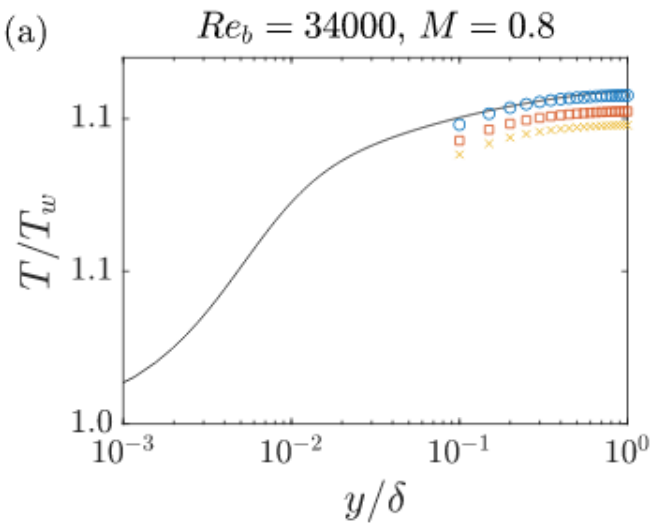
Chen, Lv, Xu, Shi, Y., & Yang, X.(2022). Physical Review Fluids, 7(1), 014608.

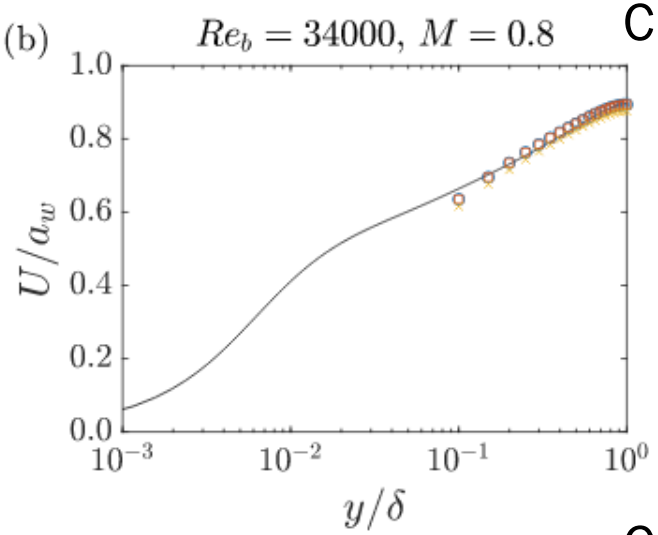
Chen, P. E., Huang, G. P., Shi, Y., Yang, X., & Lv, Y. (2022). Journal of Fluid Mechanics, 951, A38.

Huang, P. G., Coleman, G. N., Spalart, P. R., & Yang, X. (2023). Journal of Fluid Mechanics, 977, A49.

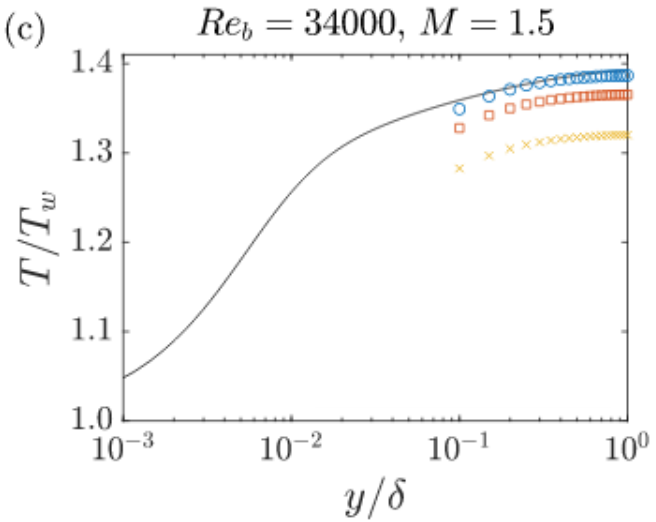
A Case Study

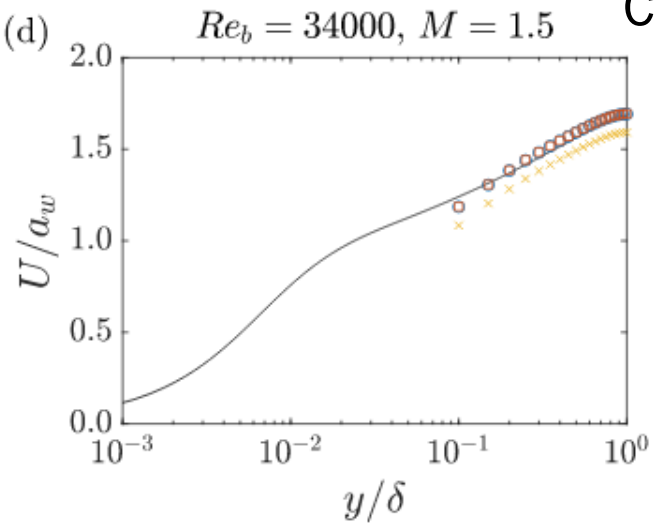
Temperature and Velocity





Cruise speed of commercial airliners





Cruise speed of fighter jets

baseline
new D, old Pr_t
new D, new Pr_t
DNS

Take-home Message

- The ODE-based WM is preferred over the algebraic WM for heat transfer problems.
- To accurate capture heat transfer, the damping function and the turbulent Prandtl number need be replaced with the following

$$D = [1 - \exp(-y^*/A^+)]^2 \qquad Pr_{t,\epsilon} = \frac{\mu_t}{\alpha_t} = \frac{\kappa}{\kappa_T} \frac{[1 - \exp(-y^*/A)]^2 + A_T\epsilon}{[1 - \exp(-y^*/A_T)]^2 + A\epsilon}$$

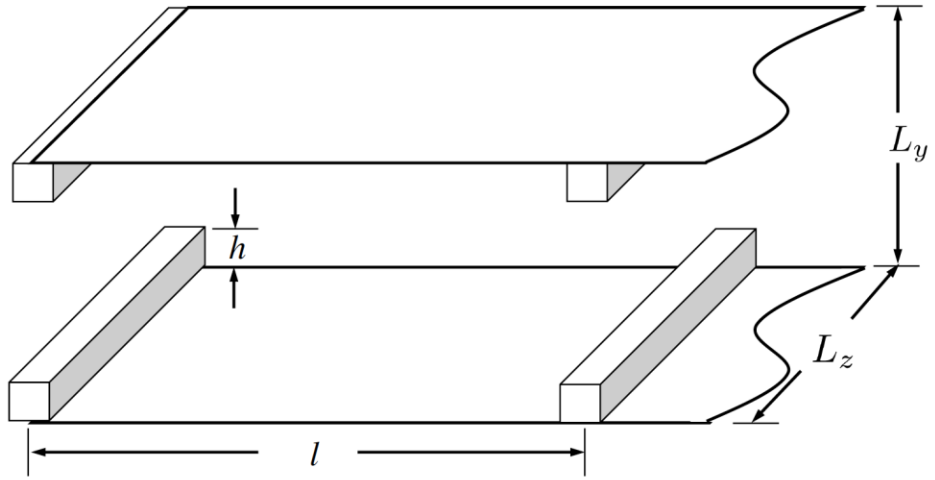
Outline of the Talk

EWM and its immediate extensions

- Surface roughness: partly resolved/unresolved surface roughness
- Heat transfer: smooth wall
- Heat transfer: fully resolved surface roughness
- Heat transfer: partly resolved surface roughness
- Pressure gradient

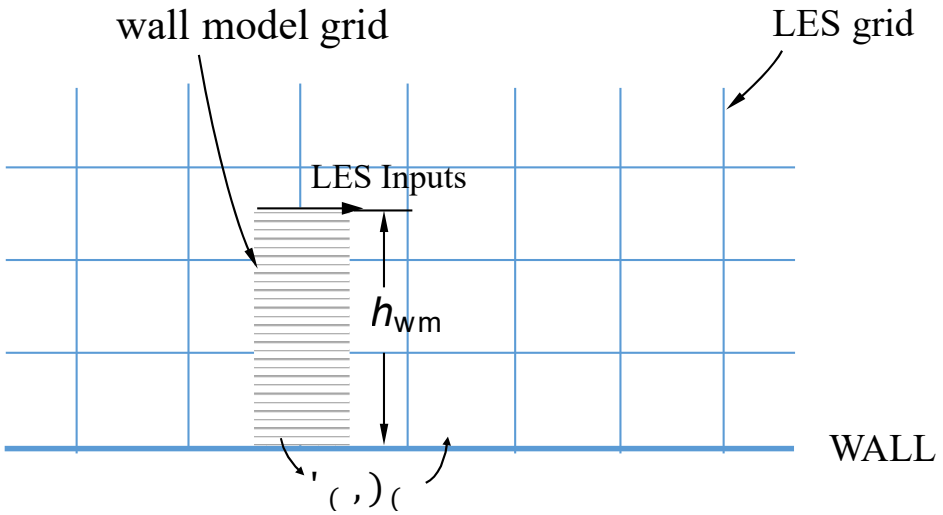
Flow Problem

Flow configuration



l = 6h, 10h, 12h

Wall Model

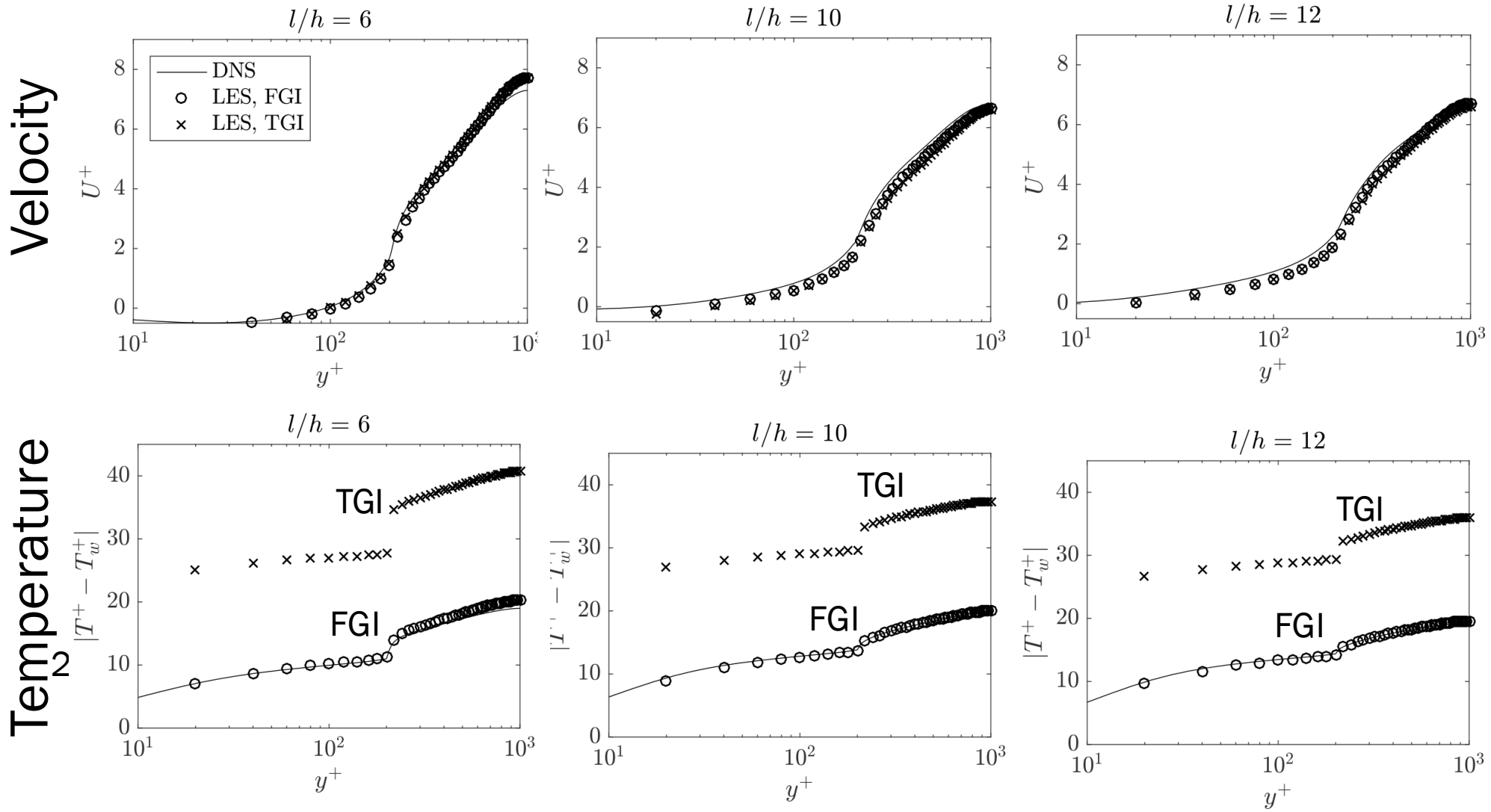


Matching location:

TGI, third grid point interfacing [Kawai & Larsson 12]

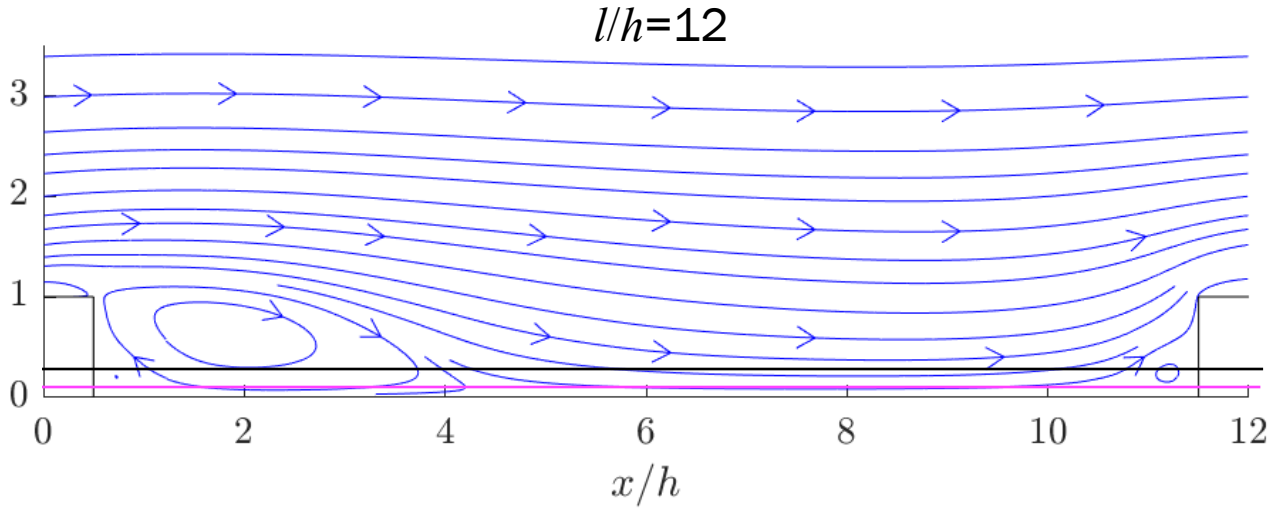
FGI, first grid point interfacing [Yang, Park, & Moin 17]

Results



TGI and FGI give the same result for velocity but different results for temperature.

Flow Physics



$$\Delta = h/10$$

WM/LES matching at 3rd point

WM/LES matching at 1st point

-- Momentum loss: form drag, wall-stress modeling is not critical.

[WMLES: good at high angles of attack, but not good at low angles of attack.]

-- Heat transfer: no pressure-like term, wall modeling critical.

-- Matching at the 1st grid point = using a finer grid.

Take-home Message

- To capture heat transfer in rough-wall TBL, we need to make good use of the available resolution in the grid by matching at the 1st grid point [by following the practice in Yang et al. 2017].

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- Heat transfer: fully resolved surface roughness
- Heat transfer: partly resolved surface roughness
- Pressure gradient

The LoW for Rough-wall TBL

Velocity, Smooth wall $U^+ = \frac{1}{\kappa}\ln(y^+) + B$

Velocity, Rough wall $U^+ = \frac{1}{\kappa}\ln(y^+) + B - \boxed{\Delta U^+}$

Temperature, Smooth wall $\Theta^+ = \frac{1}{\kappa}\ln(y^+) + B(Pr)$

Temperature, Rough wall $\Theta^+ = \frac{1}{\kappa}\ln(y^+) + B(Pr) - \boxed{\Delta\Theta^+}$

When Reynolds number is sufficiently high: fully rough regime

ΔU^+ increases as $\ln(Re_\tau)$

$\Delta\Theta^+$?? It seems that this becomes Reynolds number independent.

Heat transfer: partly resolved surface roughness

This is a missing piece:

Flow physics?

Models' behaviors?

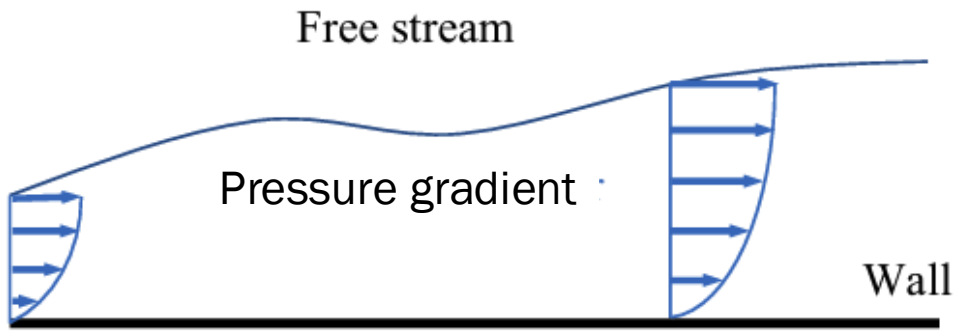
Outline of the Talk

EWM and its immediate extensions

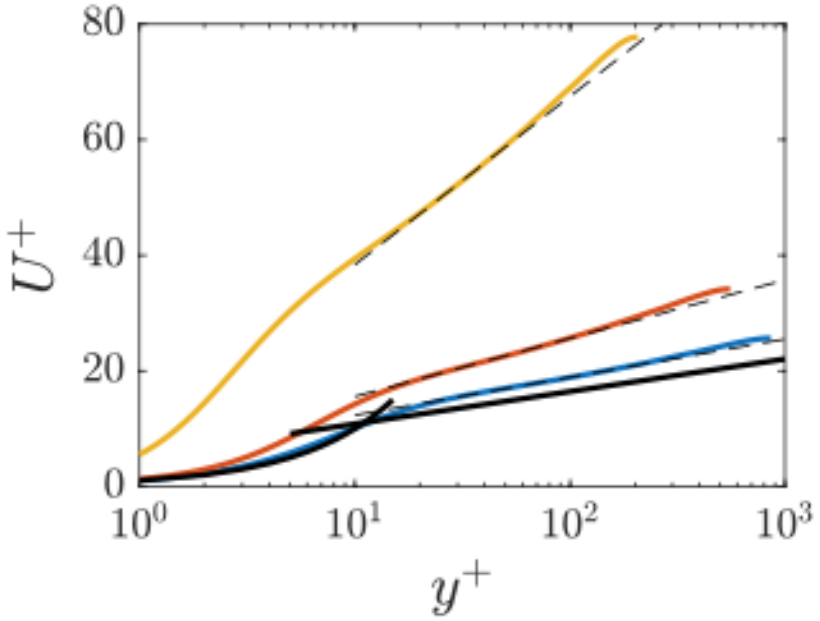
- Surface roughness: partly resolved/unresolved surface roughness
- Heat transfer: smooth wall
- Heat transfer: fully resolved surface roughness
- Heat transfer: partly resolved surface roughness
- Pressure gradient

Flow Problem

Flow configuration



Mean flow



-- The law of the wall fails.
-- Generally, there cannot be a locally-determined mean flow scaling.

-- F=ma → a=F/m=f → dV=f dt, History effects!

Near-wall Turbulence Modeling

Thin boundary-layer equation

$$\frac{\partial U}{\partial t} + U\frac{\partial U}{\partial x} + V\frac{\partial U}{\partial y} = -\frac{1}{\rho}\frac{\partial P}{\partial x} + \frac{\partial \tau_{xy}}{\partial y}, \quad \tau_{xy} = \nu\frac{\partial U}{\partial y} - \langle u'v' \rangle$$

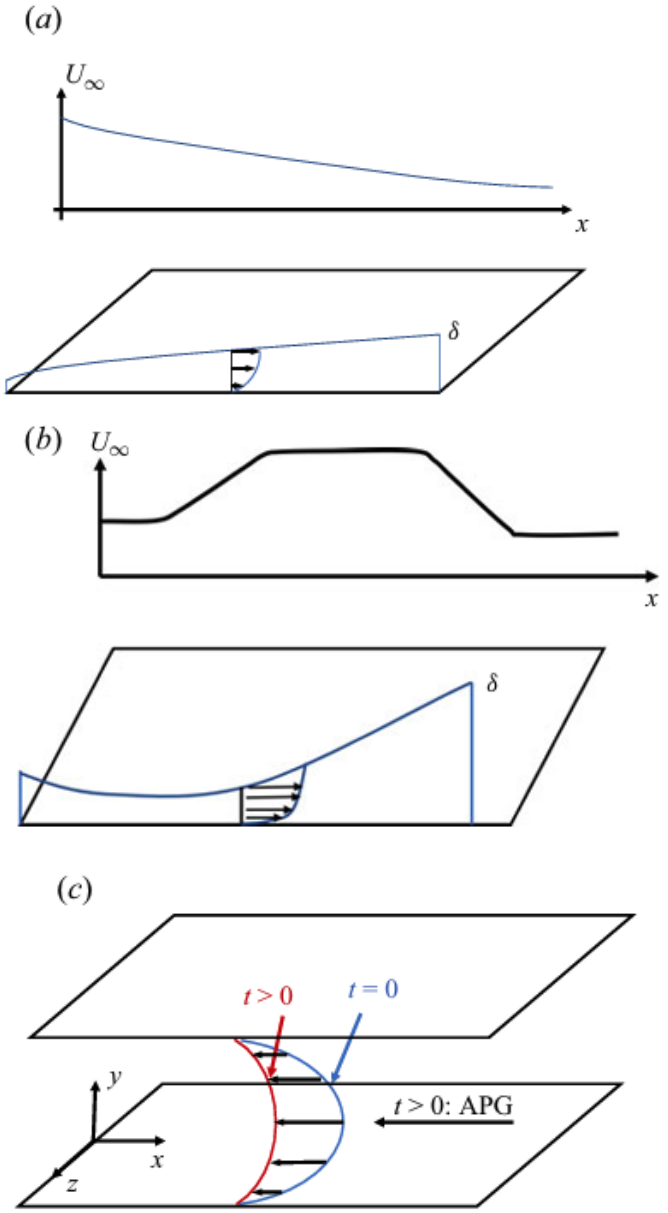
Equilibrium wall model closure: $\mu_{t,\mathrm{wm}} = \kappa\rho y\sqrt{\frac{\tau_w}{\rho}}\mathcal{D}, \quad \mathcal{D} = [1 - \exp(-y^+/A^+)]^2,$

Kays et al. 2004 model: $\mu_{t,\mathrm{wm}} = \kappa\rho y\sqrt{\frac{\tau_w}{\rho}}\mathcal{D}, \quad D_k = 1 - \exp\left(-y^+/A_k^+\right), A_k^+ = \frac{25.0}{c\mathcal{P}^+ + 1}$

A model based on a mean flow scaling that accounts history effects

Yang, X. I., Chen, P. E., Zhang, W., & Kunz, R. (2024). *Journal of Fluid Mechanics*, *993*, A1.
Chen, P. E., Wu, W., Griffin, K. P., Shi, Y., & Yang, X. I. (2023). *Journal of Fluid Mechanics*, *970*, A3.

Test Cases

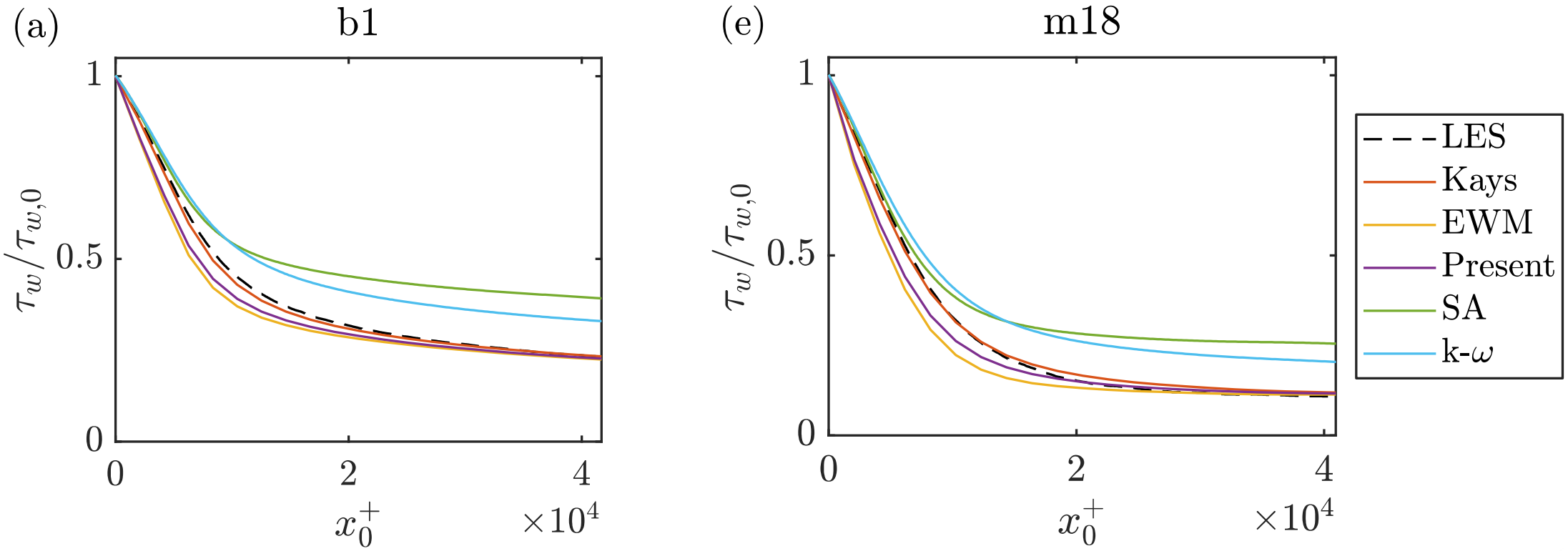


Ref.	Case name	Re_τ	Re_θ	Π	β	$p^+ \times 10^3$
Marusic & Perry (1995)	MI-A10	[1028, 1253]	[2206, 7257]	[0.0, 27.4]	[0.0, 7.16]	[0.0, 21.9]
	MI-A30	[2257, 3515]	[6430, 19133]	[0.0, 26.6]	[0.0, 6.07]	[0.0, 7.55]
Bobke *et al.* (2017)	BA-b1	[190, 862]	[910, 3360]	≈ 4.11	≈ 1	[5.1, 14.3]
	BA-b2	[189, 910]	[940, 4000]	≈ 7.55	≈ 2	[10.6, 20.8]
	BA-m13	[190, 896]	[990, 3515]	[3.80, 5.51]	[0.86, 1.49]	[5.0, 21.3]
	BA-m16	[189, 934]	[1010, 4000]	[5.82, 8.67]	[1.55, 2.55]	[10.9, 27.7]
	BA-m18	[192, 973]	[990, 4320]	[7.29, 12.5]	[2.15, 4.07]	[16.0, 33.6]
Volino (2020)	VR-case1	[304, 651]	[721, 3291]	[−7.39, 22.2]	[−0.91, 5.97]	[−17.7, 34.8]
	VR-case2	[592, 1132]	[1583, 6255]	[−8.35, 25.5]	[−1.15, 6.60]	[−11.6, 22.3]
	VR-case3	[347, 651]	[877, 2215]	[−4.41, 5.55]	[−0.57, 1.09]	[−9.2, 8.4]
	VR-case4	[570, 1072]	[1578, 3846]	[−4.66, 5.35]	[−0.58, 1.02]	[−6.2, 4.9]
	VR-case5	[955, 1875]	[2947, 7142]	[−4.48, 6.02]	[−0.65, 1.11]	[−3.9, 3.2]
	VR-case6	[260, 686]	[673, 2122]	[−2.15, 2.53]	[−0.24, 0.46]	[−4.8, 3.6]
	VR-case7	[574, 1170]	[1541, 3891]	[−2.53, 2.71]	[−0.28, 0.48]	[−3.2, 2.3]
	VR-case8	[931, 1901]	[2765, 6386]	[−2.45, 2.51]	[−0.30, 0.42]	[−1.9, 1.3]
Pozuelo *et al.* (2022)	PR-b1.4	[800, 1900]	[3700, 8700]	[5.39, 6.49]	[1.20, 1.65]	[2.8, 8.1]
Chen *et al.* (2023)	CP-R5A1	[544, 0]	[1008, 143]	[1, ∞]	[0.13, ∞]	[1.84, ∞]
	CP-R5A10	[544, 0]	[1008, 537]	[10, ∞]	[1.31, ∞]	[18.4, ∞]
	CP-R5A100	[544, 0]	[1008, 957]	[100, ∞]	[19.9, ∞]	[184, ∞]
	CP-R10A10	[1000, 0]	[1927, 1085]	[10, ∞]	[1.15, ∞]	[10.0, ∞]
	CP-R10A100	[1000, 0]	[1927, 1777]	[100, ∞]	[11.5, ∞]	[100, ∞]

Table 1. Details of the data in Marusic & Perry (1995), Bobke *et al.* (2017), Pozuelo *et al.* (2022), Volino (2020) and Chen *et al.* (2023).

Results

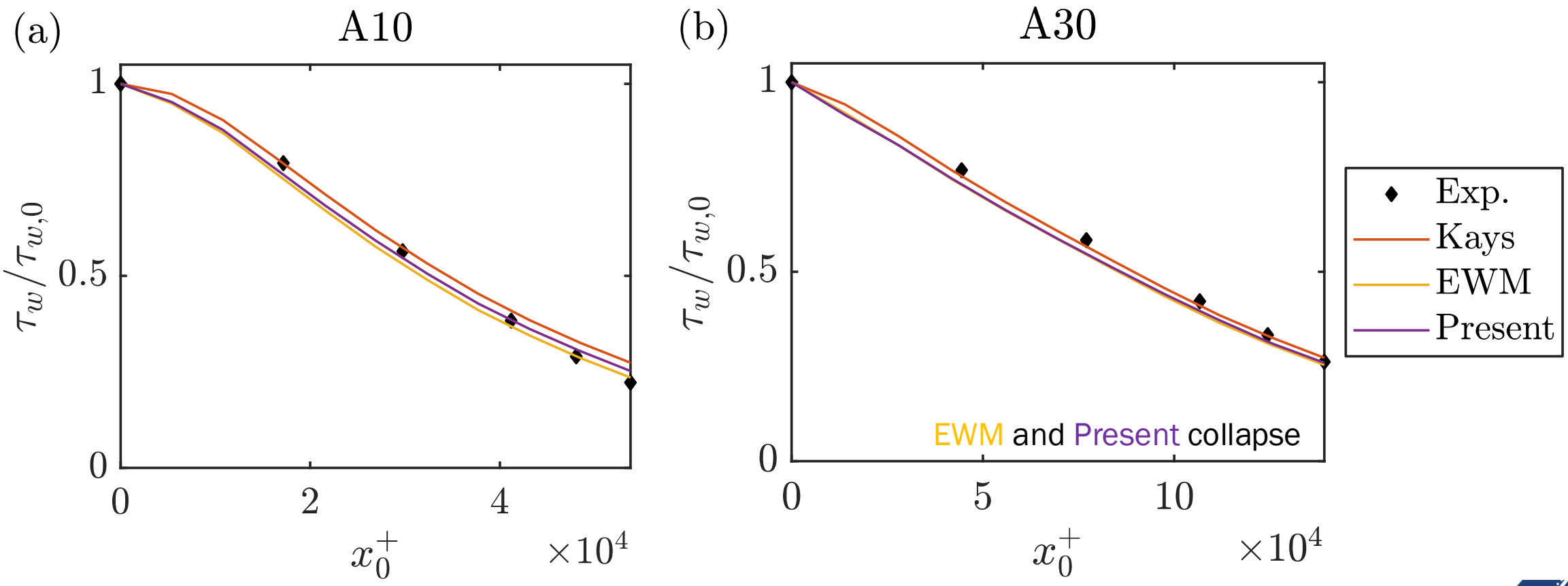
Bobke et al 2017, moderate PG



Kays > EWM ≈ Present ≫ SA ≫ k − ω

Results

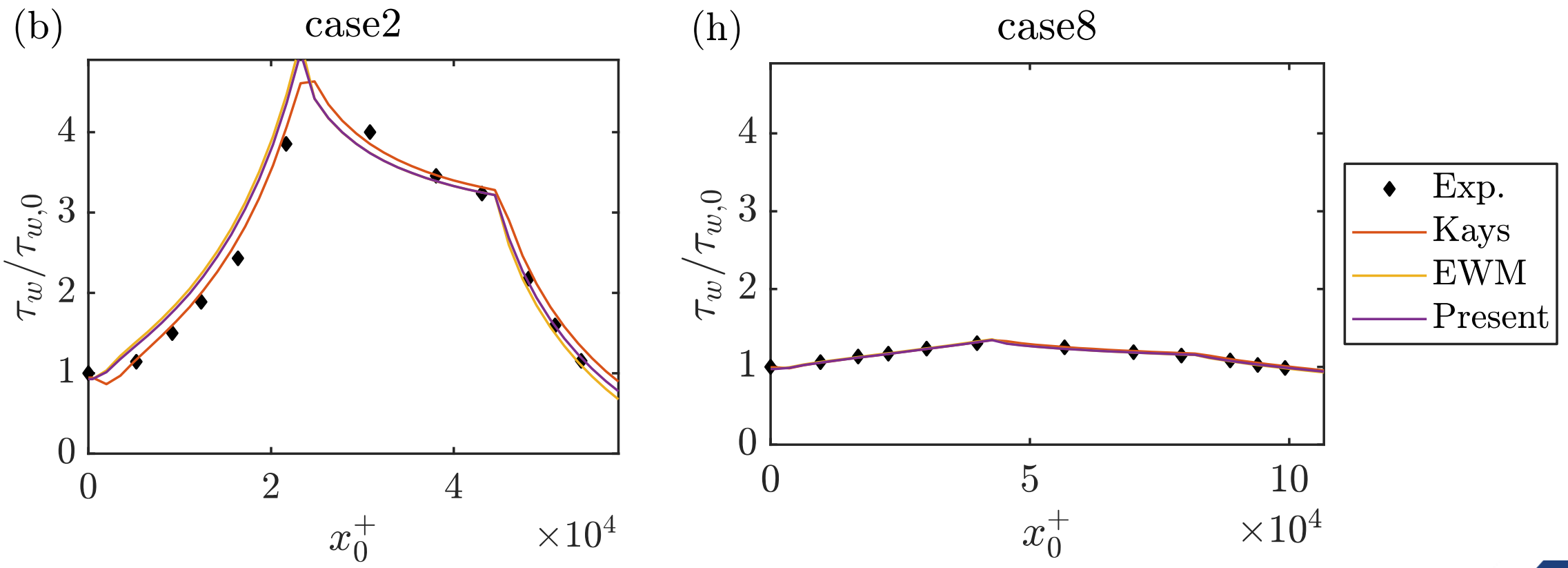
Marusic & Perry 1995, moderate PG



Kays ≈ EWM ≈ Present

Results

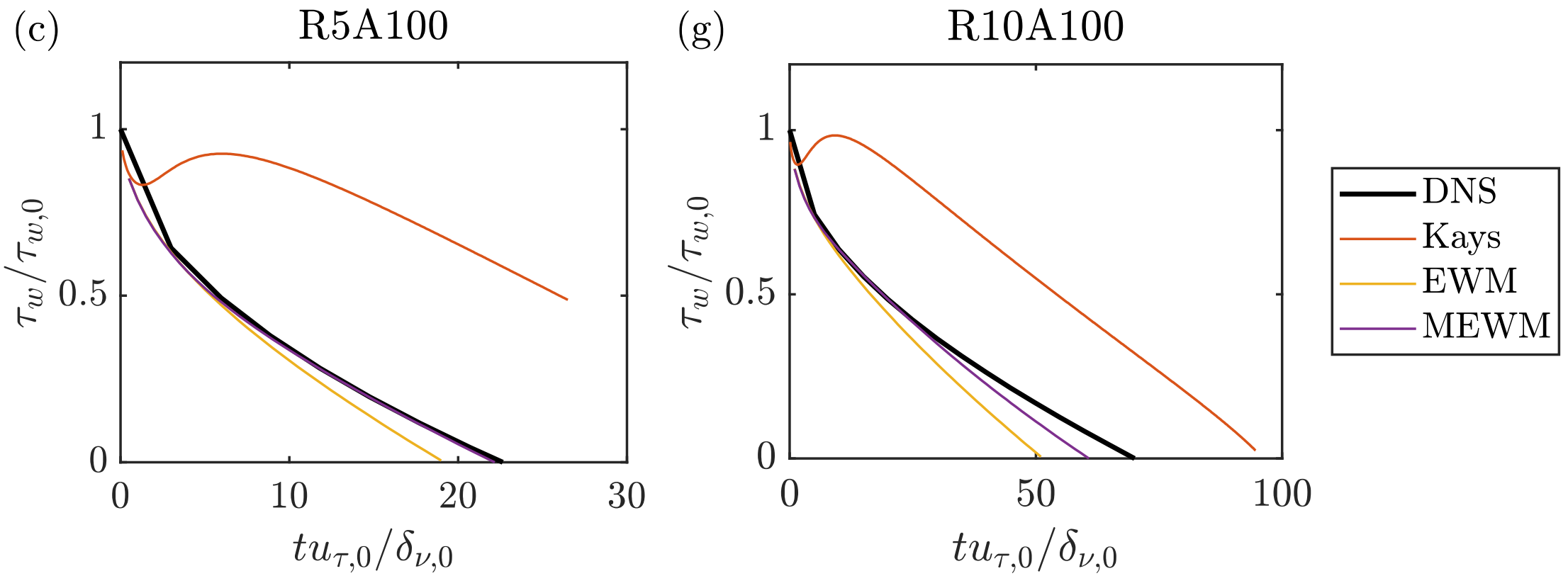
Volino 2020, moderate PG



Kays ≈ EWM ≈ Present

Results

Chen et al. 2023, strong PG



Present > EWM > Kays

Take-home Message

- By including the material derivative, the EWM accounts for pressure gradients.

The pieces of a puzzle

EWM and its immediate extensions

– Roughness modeling

– Finite Mach number

– Matching location

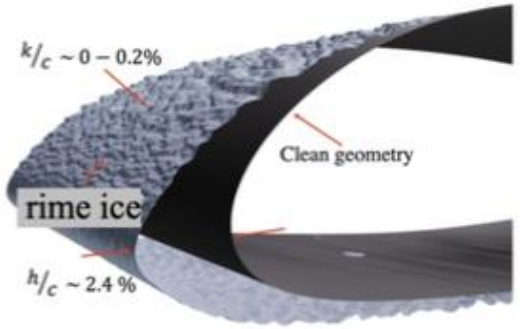
– Material derivative term

Putting these pieces together for the icing problem.

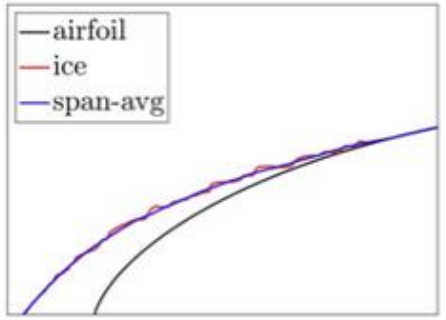
Icing: Approach

Real world roughness → Unwrap to a flat plate geometry

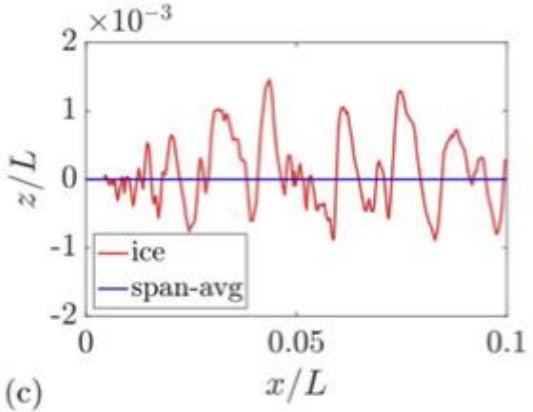
- Roughness
- Pressure gradient
- Heat transfer
- …



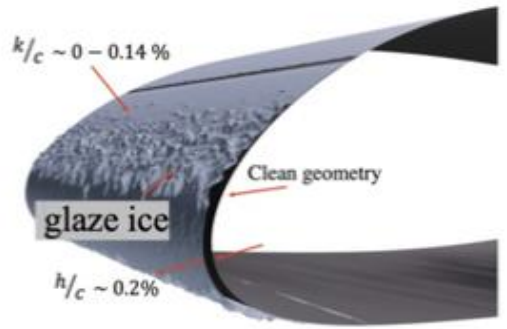
(a)



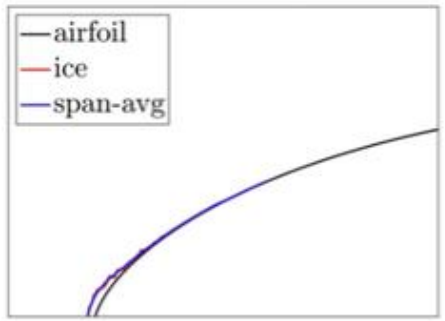
(b)



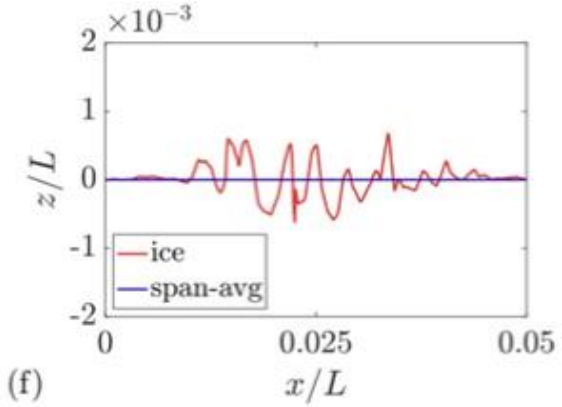
(c)



(d)



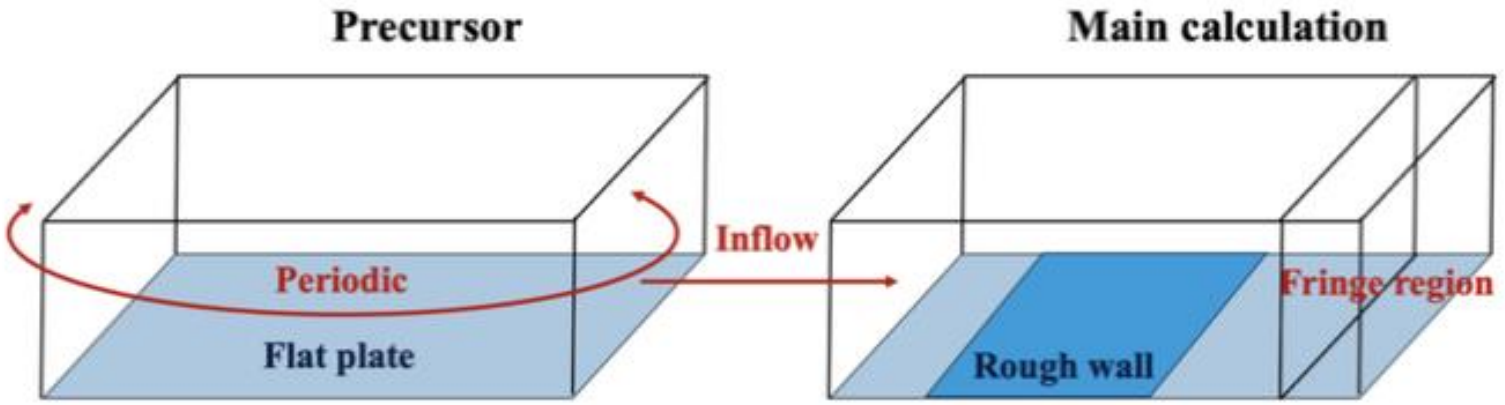
(e)



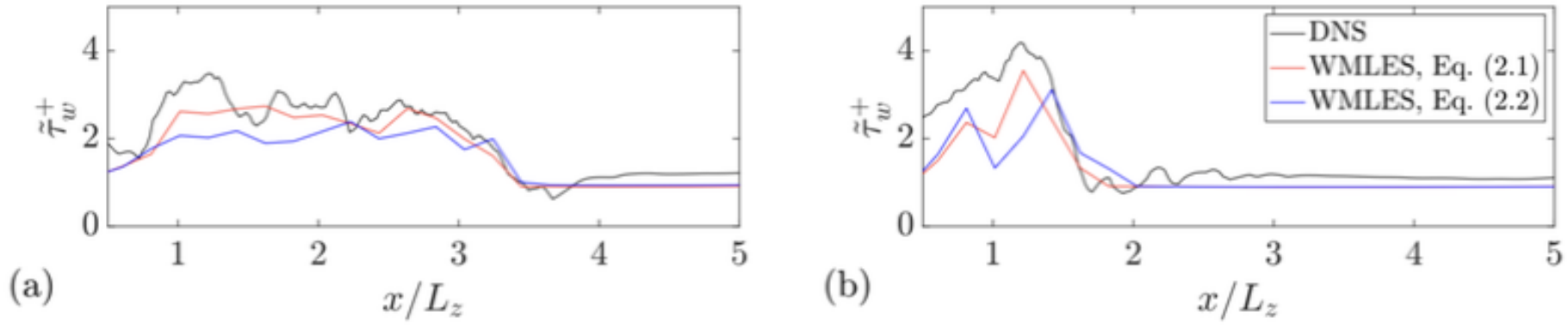
(f)

Icing: Roughness

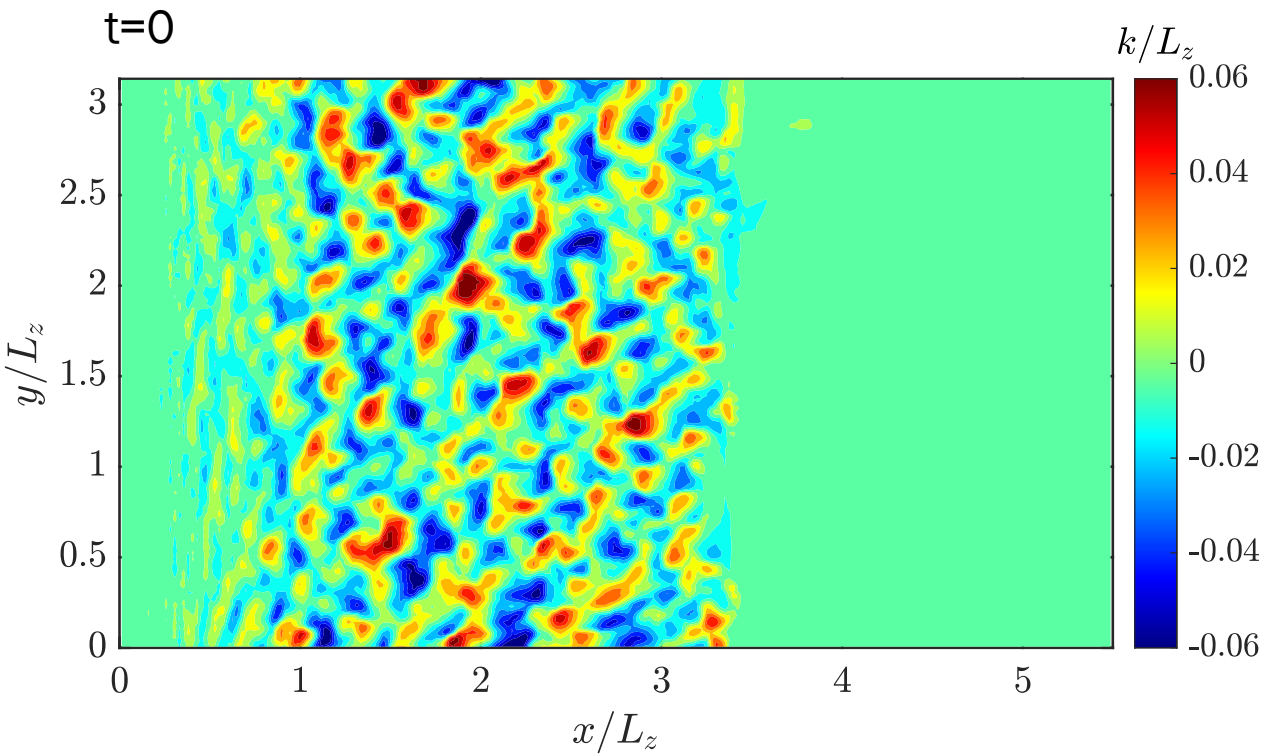
Flow Setup

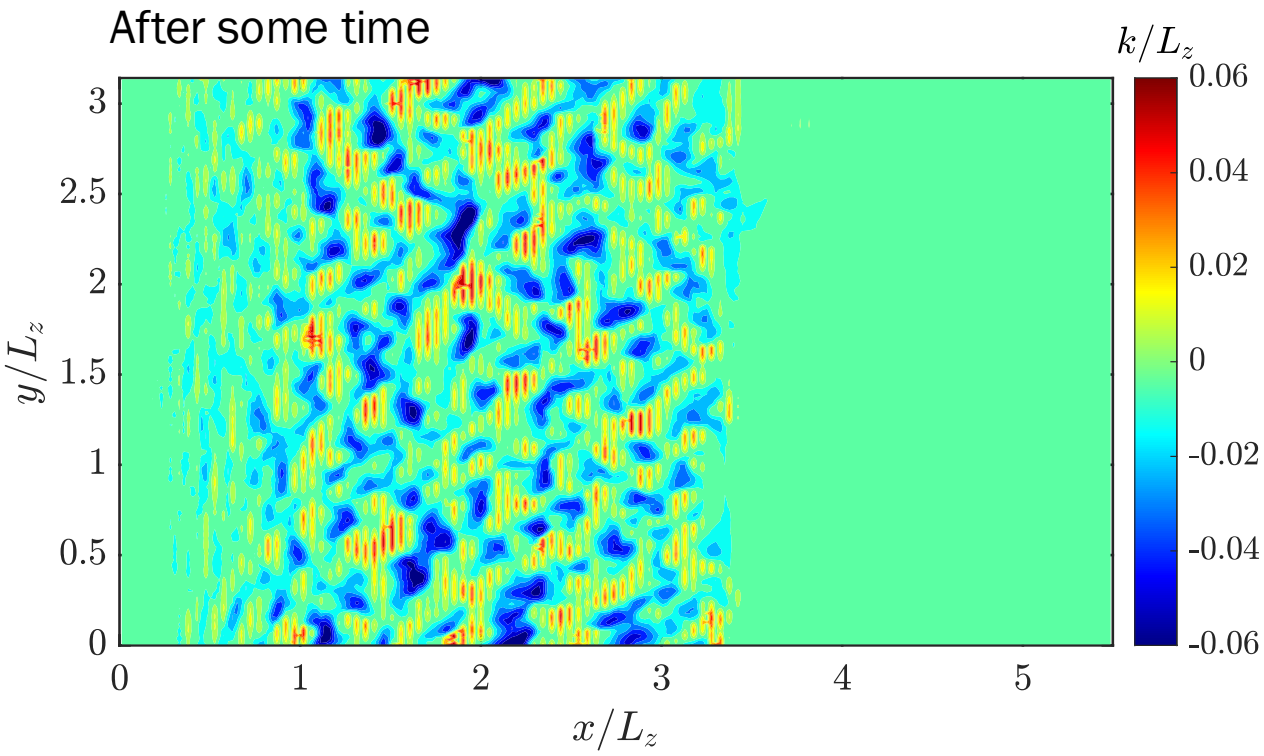


WMLES



Icing: Phase Change





DNS on-going...

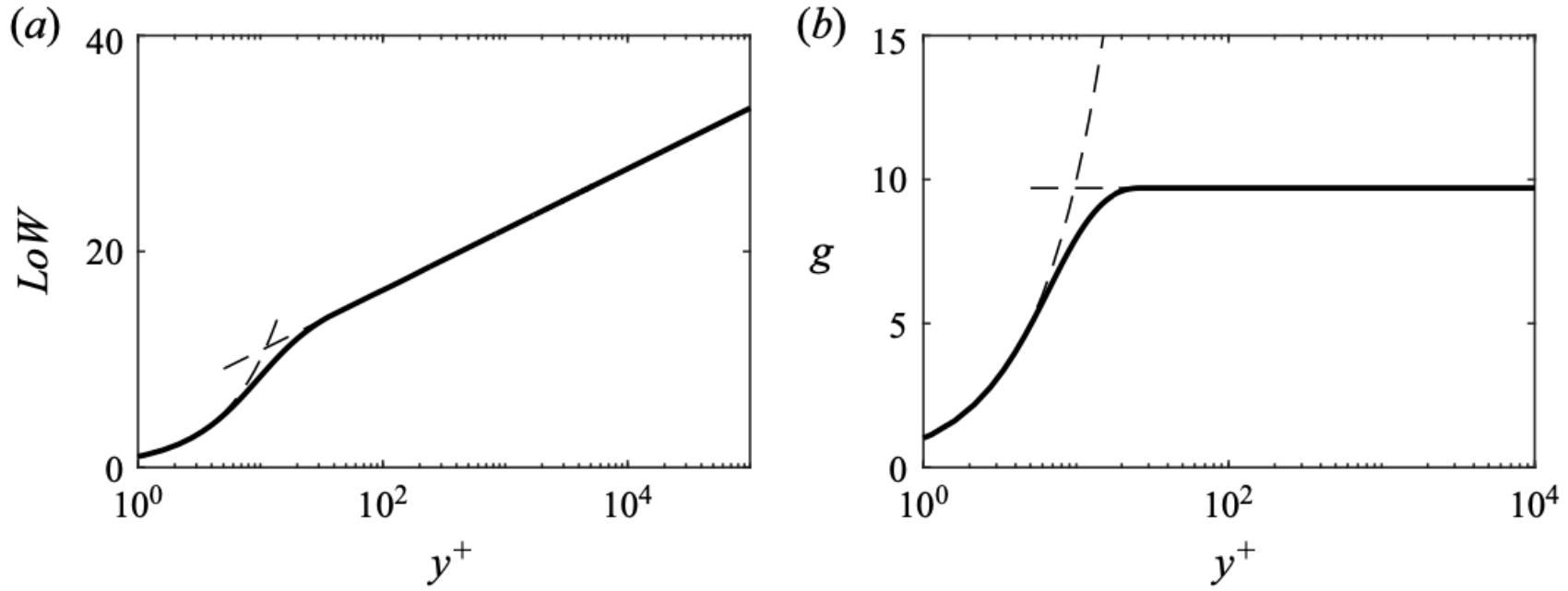
Hu, X., Agrawal, R., Zabaleta, F., Bornhoft, B., & Yang, X. I. A. Flow over ice roughness Part II. Heat transfer and pressure gradient, CTR, ARB.
Hu, X., Agrawal, R., Zabaleta, F., Bornhoft, B., & Yang, X. I. A. Flow over ice roughness Part II. Heat transfer and pressure gradient, CTRSP.

FPCRL at Penn State

- Wall modeling in high-order codes
- Generalizable data-driven ML models
- Data-enabled convergence accelerator
- Data-enabled fast prediction

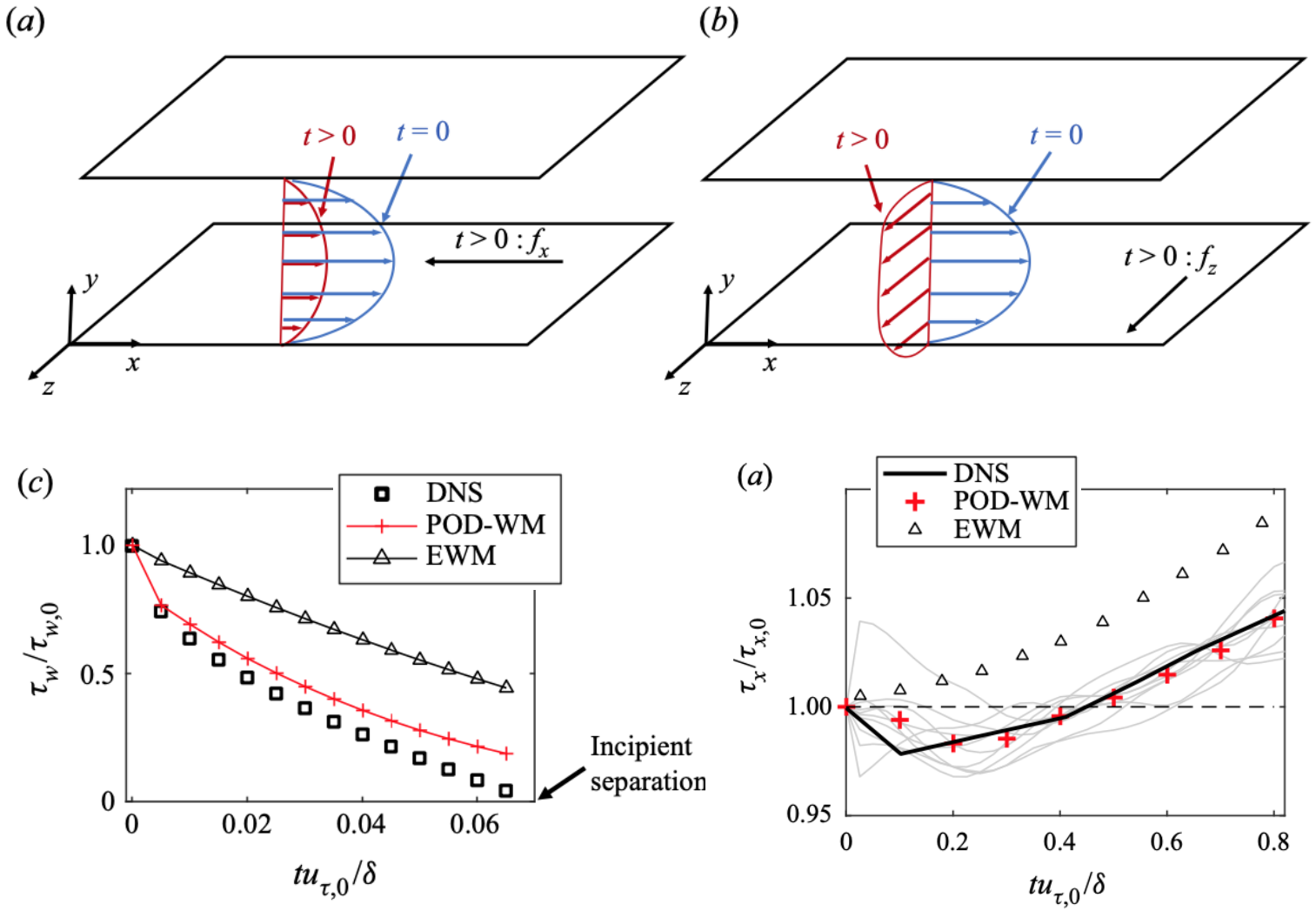
High-order Reconstruction of Wall Layer

Unresolved Wall Layer = Law of the wall + another mode (from, e.g., POD analysis)



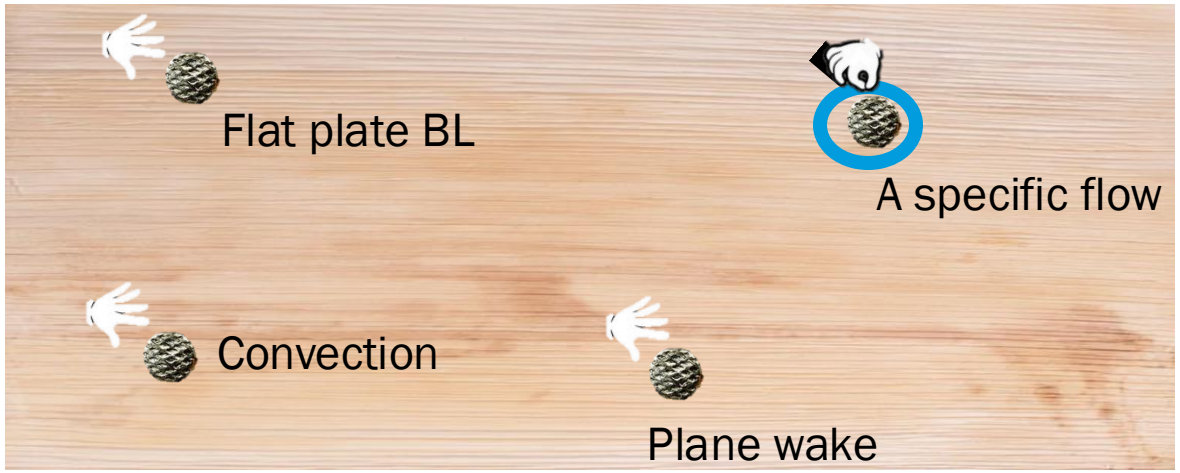
Hansen, Abkar, & Yang, (2023), J Fluid Mech, 975, A24
Hansen, Sørensen, Yang, & Abkar, (2024). Physics of Fluids, 36(1).

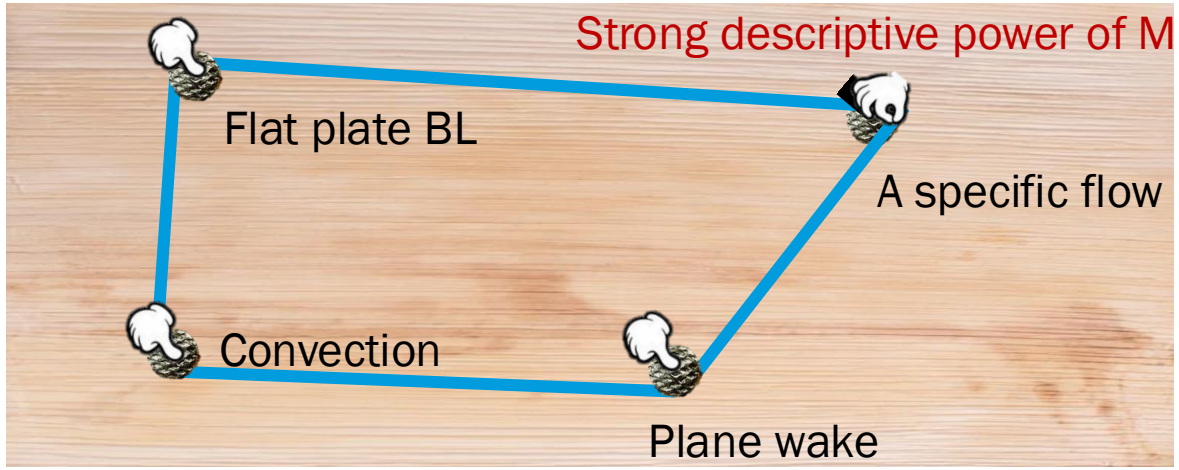
High-order Wall Model in High-order Codes



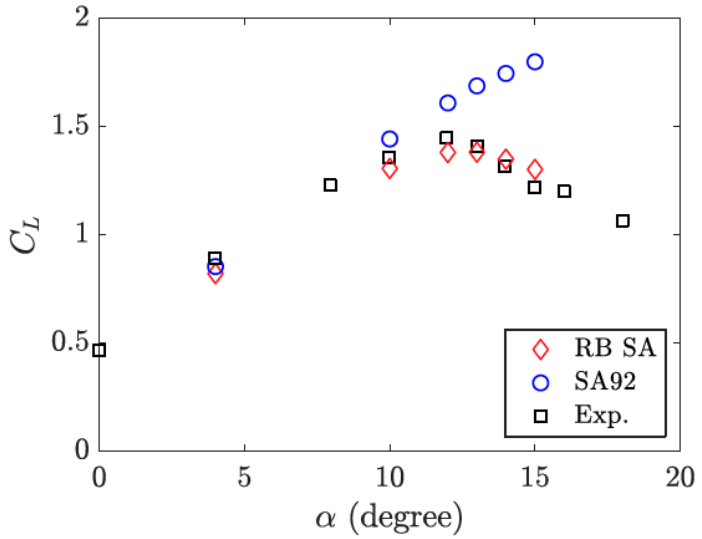
High-order methods holds great potential for WMLES.

Rubber-band Approach to Data-driven Models





Generalizable Prediction of Stall

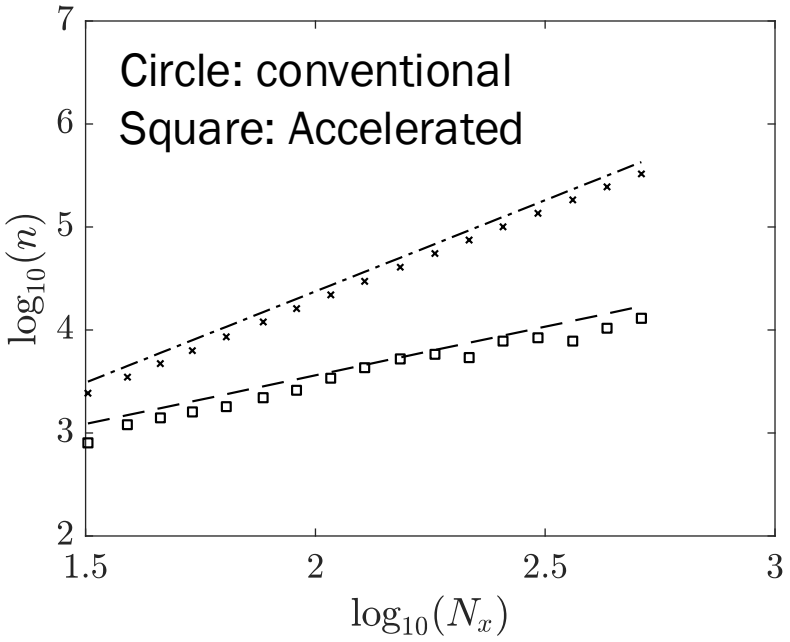


Bin, Chen, Huang, Yang (2022). *Phys. Rev. Fluids*, 7(8), 084610.
Bin, Hu, Li, Grauer, Yang (2024). *Theor. Appl. Mech. Lett.*, 14(2), 100503.
Yang, Zafar, Wang, Xiao (2019). *Phys. Rev. Fluids*, 4(3), 034602.
Huang, Yang, Kunz (2019). *Phys. Fluids*, 31(12).
Huang, Yang (2021). *Phys. Fluids*, 33(1).
Wang, Yang, Ovchinnikov (2024). *J. Atmos. Sci.*, 81(2), 435–458.
Bin, Huang, Yang (2023). *AIAA J.*, 61(11), 4852–4863.
Bin, Huang, Kunz, Yang (2024). *AIAA J.*, 62(4), 1434–1446.

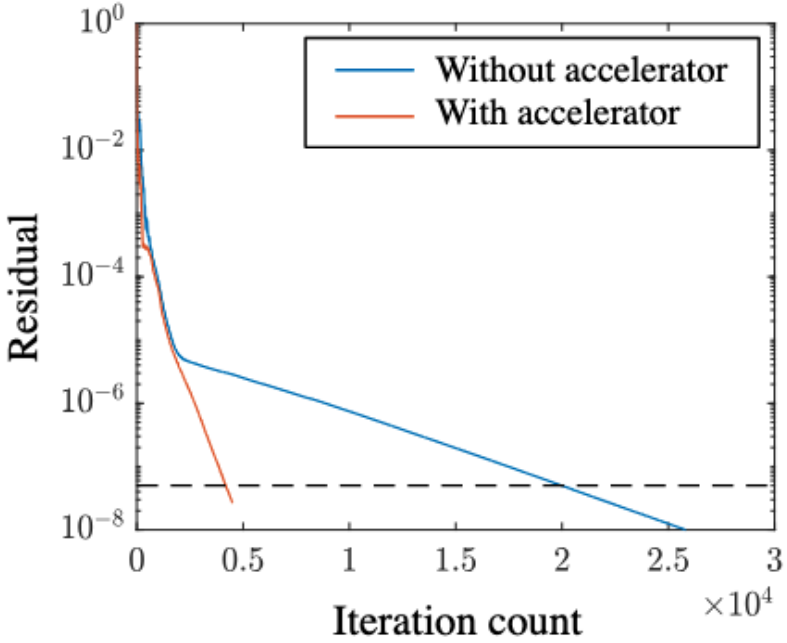
Data-enabled Convergence Accelerator

Periodically project the residual to a reduced-order space

Reduction of time complexity



OpenFOAM, Periodic Hill



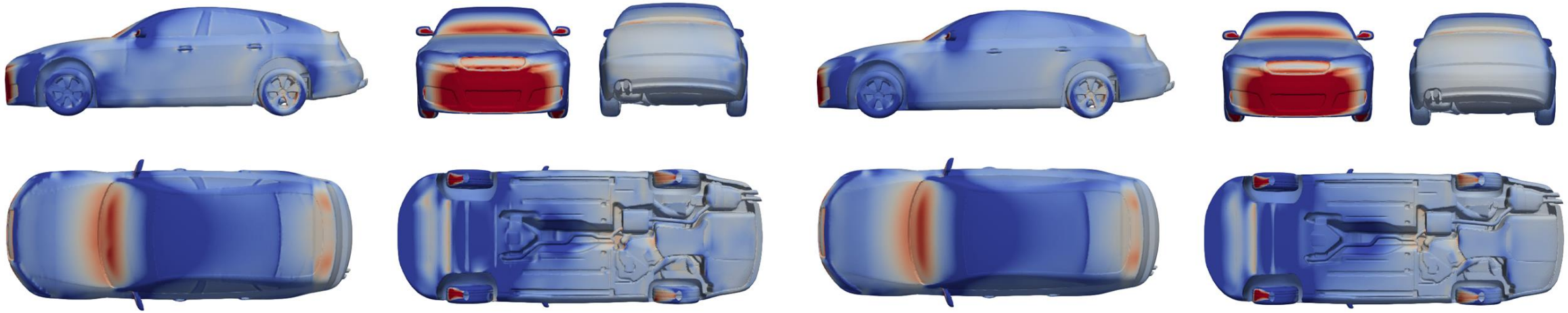
O(3-10) acceleration

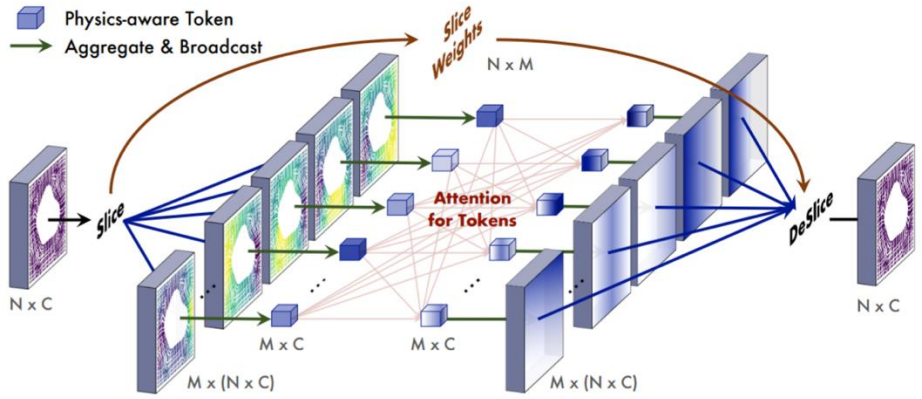
Bin, Y., Yang, X. I., Grauer, S. J., & Kunz, R. F. (2025). Data-enabled reduction of the time complexity of iterative solvers. *Journal of Computational Physics*, *529*, 113859.

Data-enabled Fast Prediction

Truth

ML





Prediction in seconds.

Thanks for your attention!

xzy48@psu.edu