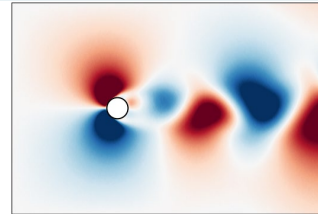
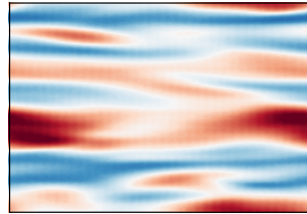
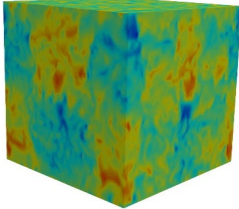
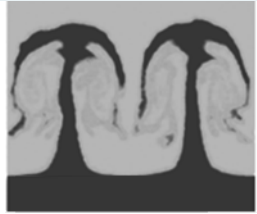




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Molecular-level simulations of turbulent Couette flow over a thermal-protection-system material



Ryan M. McMullen¹, Arnaud Borner², Michael A. Gallis¹

¹Sandia National Laboratories

²AMA, Inc. at NASA Ames Research Center

DSMC25

Santa Fe, New Mexico, USA

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Turbulent flow over TPS materials



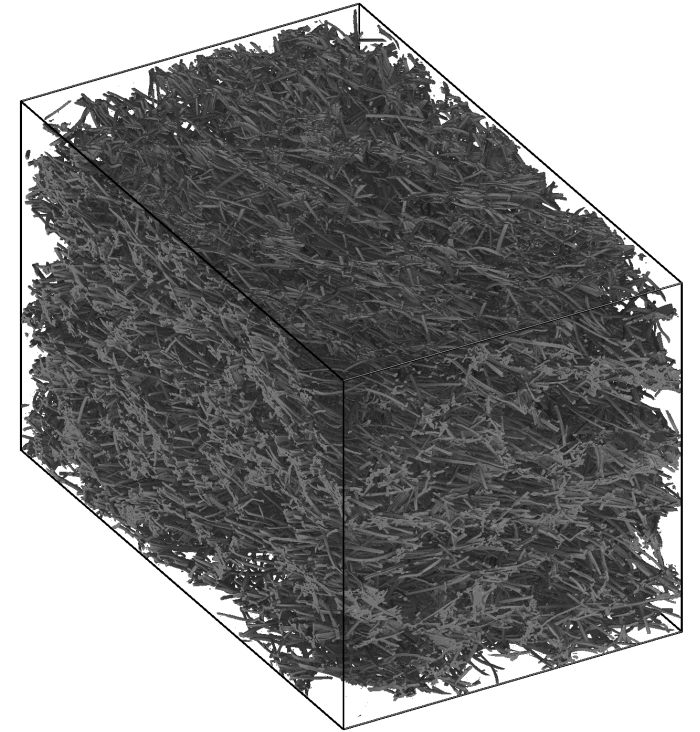
Thermal-protection-system (TPS) materials on reentry vehicles may be:

- Rough
- Permeable

Surface conditions affect aerothermal loading and may compromise vehicle performance

Simulating flow over these materials is challenging for traditional computational fluid dynamics (CFD)

- Substrate geometries can be difficult to mesh
- Noncontinuum effects may be significant within the substrate



3D scan of FiberForm™

DSMC *should* be well suited for simulating turbulence over TPS materials!

But first: can DSMC simulate wall-bounded turbulence?



DSMC faithfully simulates decaying turbulence in a periodic box ...
What about when the flow is driven by solid boundaries?

- Gas-surface interactions are also important
- Can DSMC reproduce the self-sustaining cycle of wall-bounded flows? [1]

Simulate smooth-wall turbulent Couette flow at different Re [2]:

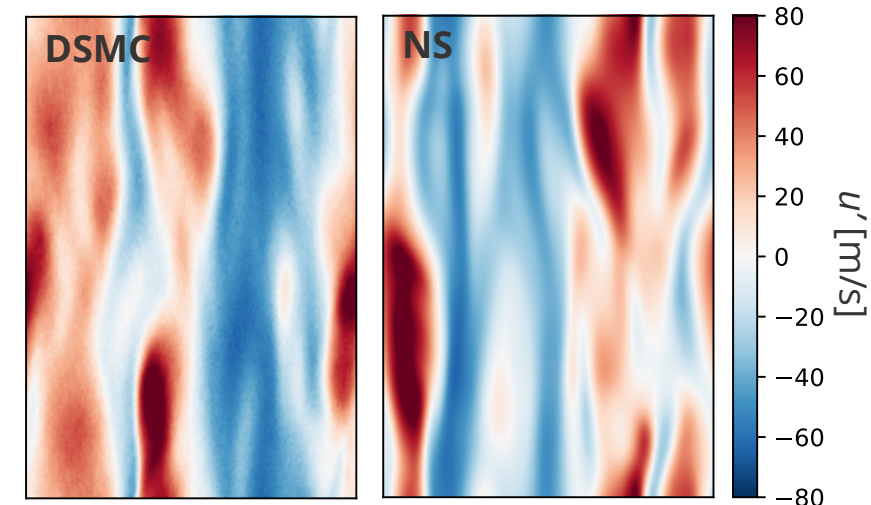
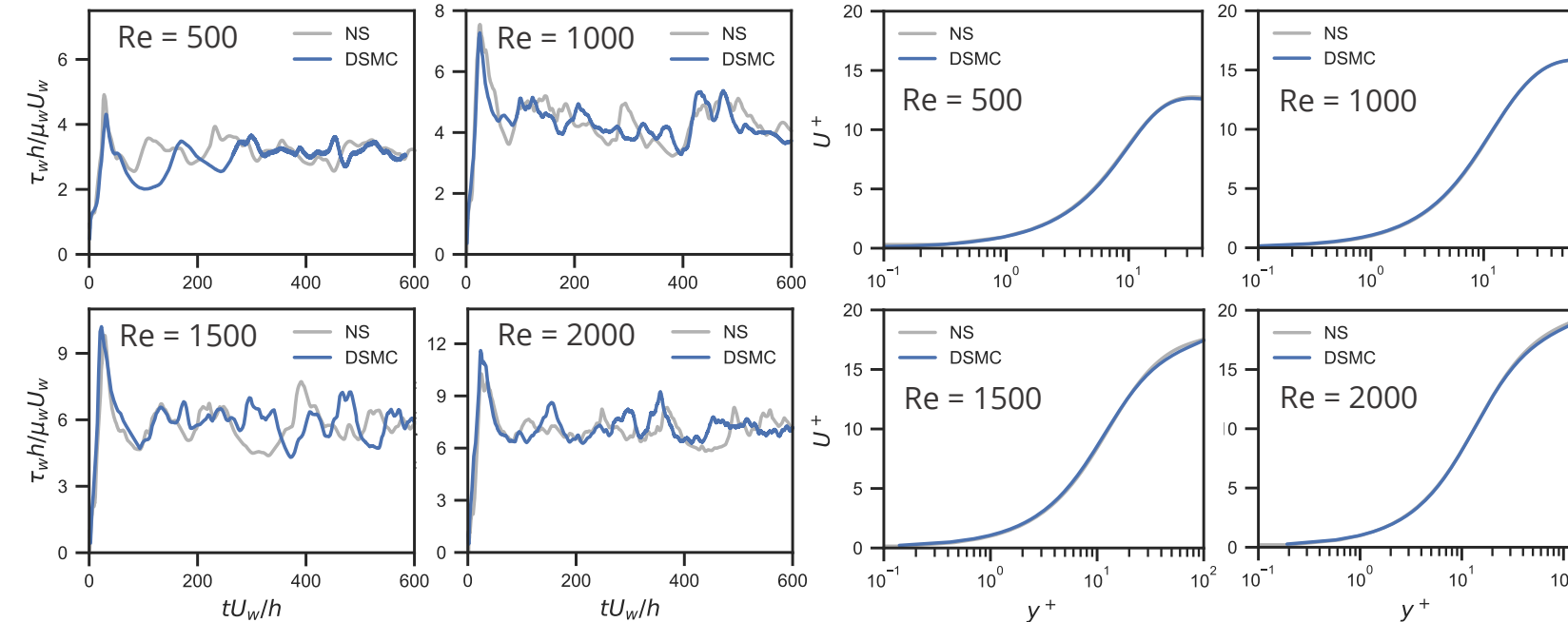


Couette flow

Skin friction

Mean velocity

Turbulence structures



$$U^+ = U / u_\tau, \quad y^+ = \rho u_\tau y / \mu;$$

$$u_\tau = \sqrt{\tau_w / \rho}$$

DSMC accurately simulates wall-bounded turbulence!

[1] Gallis et al., PRF (2018)

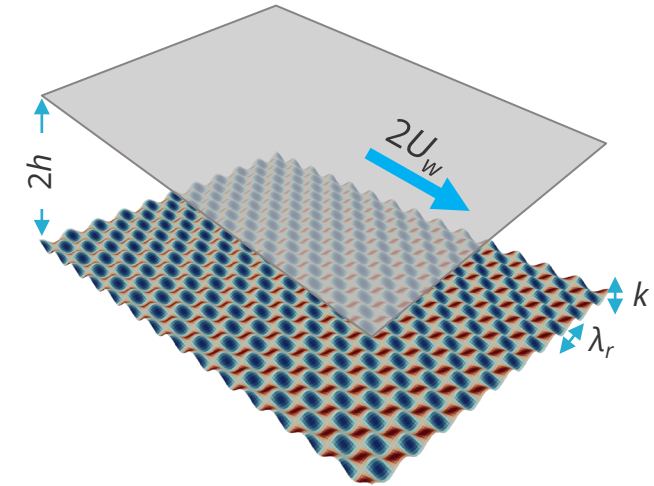
[2] McMullen et al., PRF (2023)

What about rough-wall turbulence?

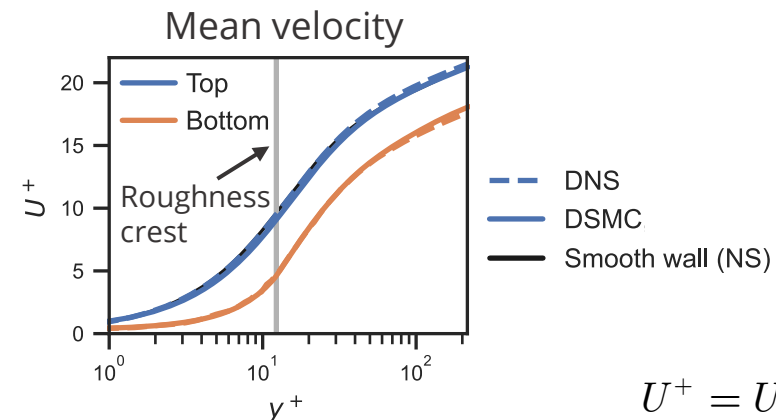
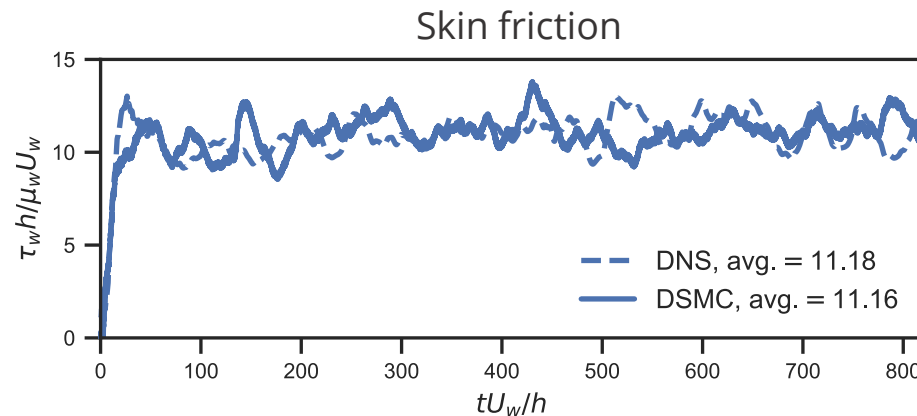


Replace bottom wall with a sinusoidal “egg carton” surface

- $Ma_0 = 1.5$, $Re_0 = 2800$
- $k/h = 1/18$, $\lambda_r/k = 7$
- Flow is in the “transitionally rough” regime
- Significant roughness effects confined to bottom half of channel (roughness modifies upper-wall turbulence through τ_w)



“Egg carton” surface



$$U^+ = U / u_\tau, \quad y^+ = \rho u_\tau y / \mu;$$

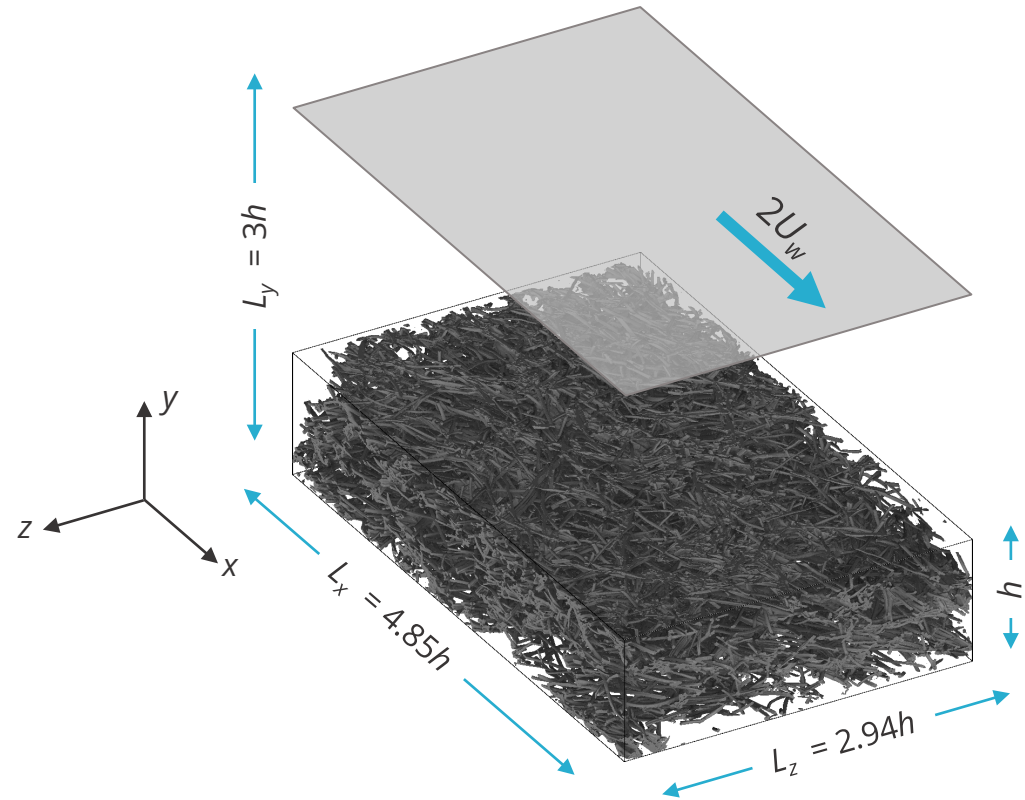
$$u_\tau = \sqrt{\tau_w / \rho}$$

DSMC accurately simulates rough-wall turbulence!

Turbulent Couette flow over TPS material



- Length scale: $h = 500 \mu\text{m}$
- Cell size: $1.65 \mu\text{m}$
- Total cells: 1.19×10^9
- Total particles: 34×10^9
- Avg. particles per cell: 30
- Time step: 9.12 ps
- Monatomic gas: $\gamma = 5/3$
- Molecular mass: $6.63 \times 10^{-26} \text{ kg}$
- Walls: diffuse reflections, $\alpha = 1$, $T_0 = 273.15 \text{ K}$
- Periodic in x and z directions



Ma_0	Re_0	Kn_0
1.5	2800	8.7×10^{-4}
3.0	5600	

$$Ma_0 = U_w/a_0$$

$$Re_0 = \rho_0 U_w h / \mu_0$$

$$Kn_0 = \lambda_0 / h$$

FiberForm substrate



FiberForm is the substrate for NASA's PICA TPS

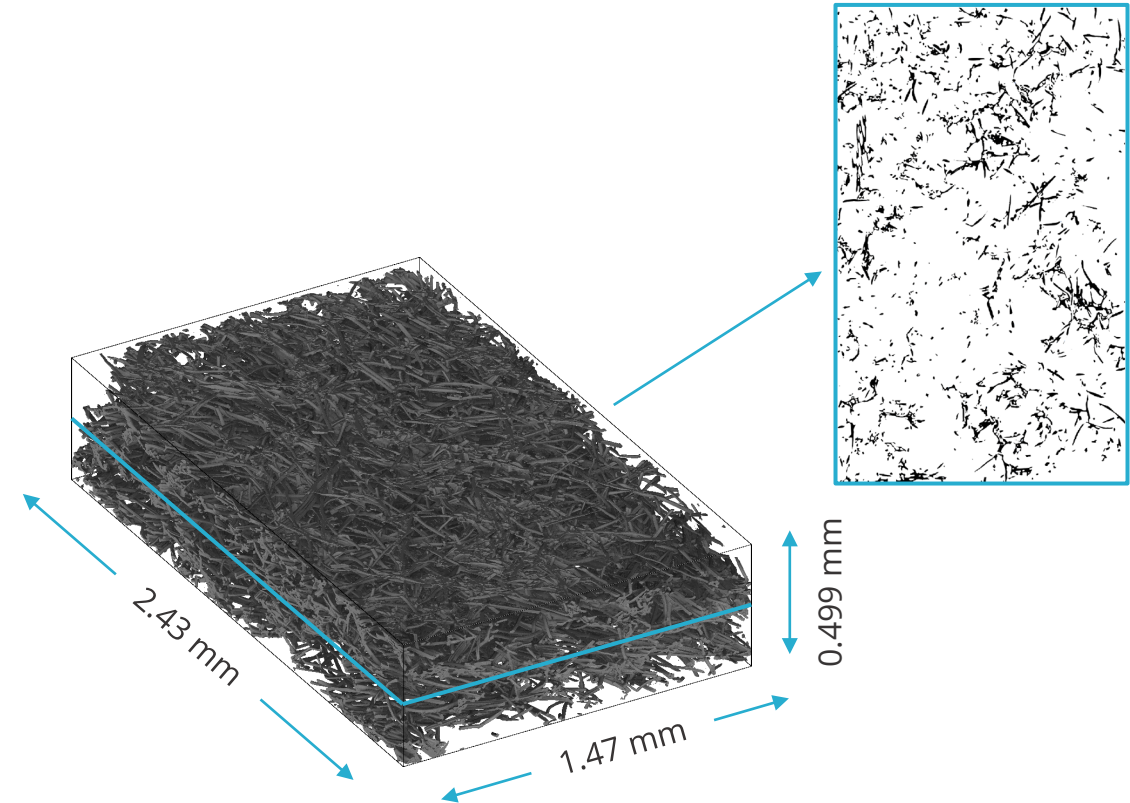
- Porosity: 0.86
- Fiber diameter: $\sim 10\ \mu\text{m}$
- Mean pore diameter: $\sim 50\ \mu\text{m}$

Image produced from μ -CT scan of real FiberForm sample

- Voxel size: $1.65\ \mu\text{m}$
- Void-phase voxels (0), solid-phase voxels (255)

SPARTA creates an *implicit surface* from the image file

- Each voxel value assigned to grid point
- Marching Cubes algorithm determines triangular surface element vertex locations from grid point values
- Creates water-tight surface that is handled the same as an explicit surface (e.g., defined by an STL file)



SPARTA enables pore-scale-resolved turbulence simulations over a real material sample!

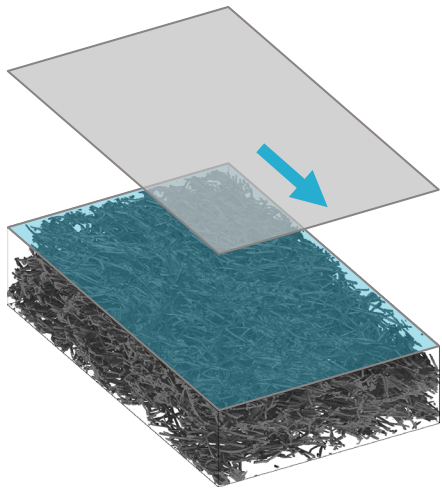
Substrate strongly modifies near-surface flow



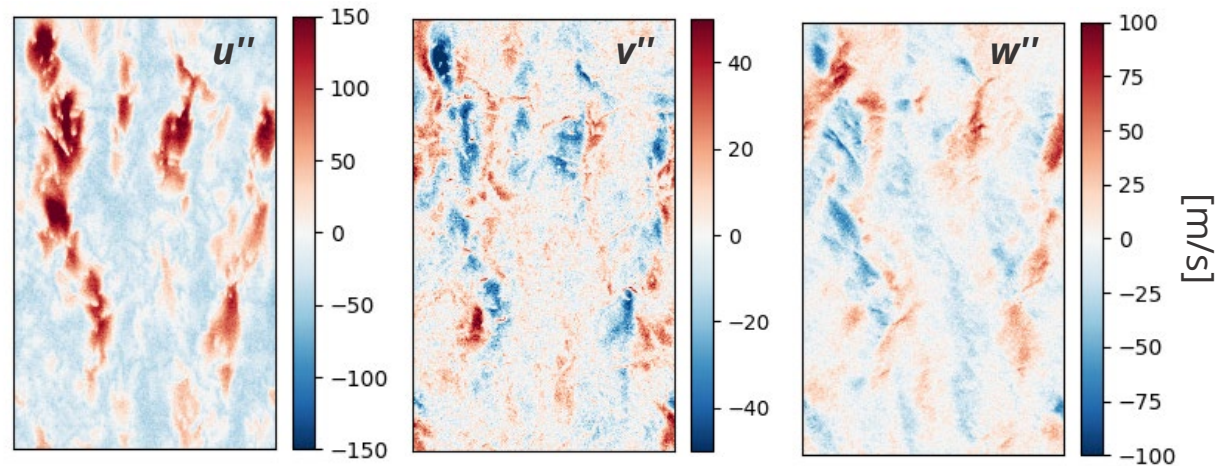
On an impermeable (smooth or rough) wall, the velocity goes to zero (no-slip condition)

Permeable substrates like FiberForm exhibit significant surface and sub-surface flow

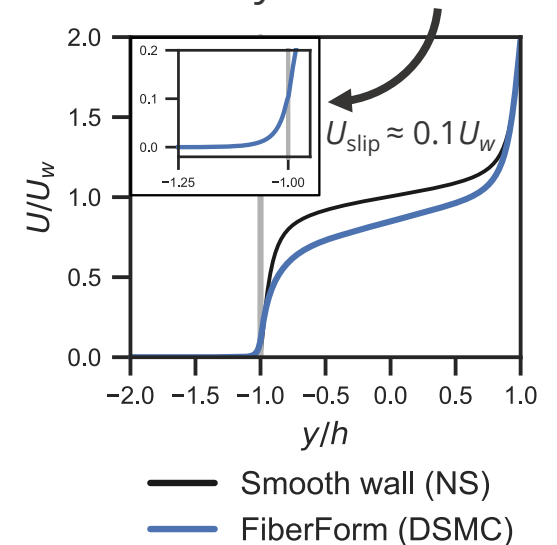
Properly accounting for flow-substrate interactions is crucial for accurately predicting engineering quantities of interest (drag, heat flux, ...)



Turbulent fluctuations at the surface



Significant mean “slip” velocity at surface



DSMC accurately resolves complex flow-substrate interactions!

Permeable surfaces increase drag

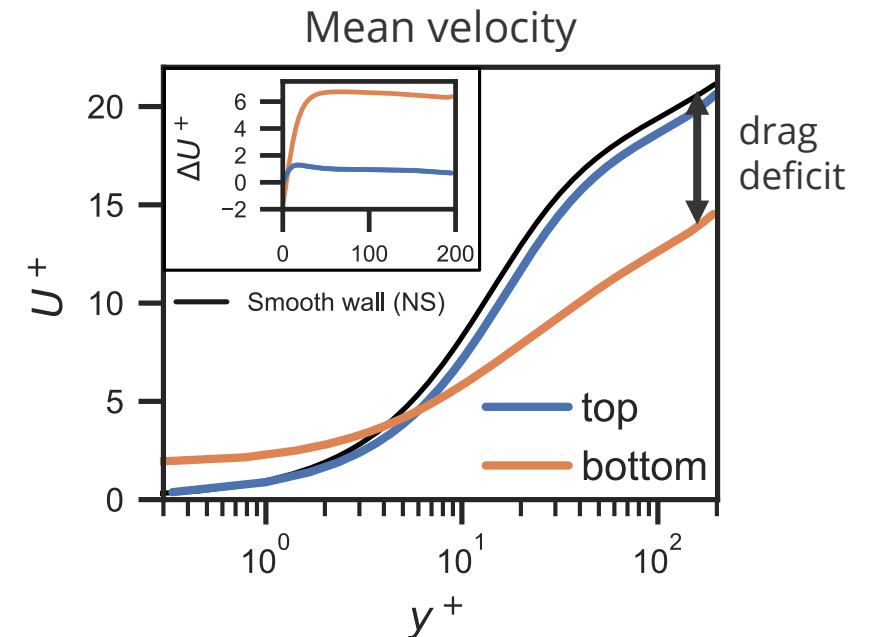
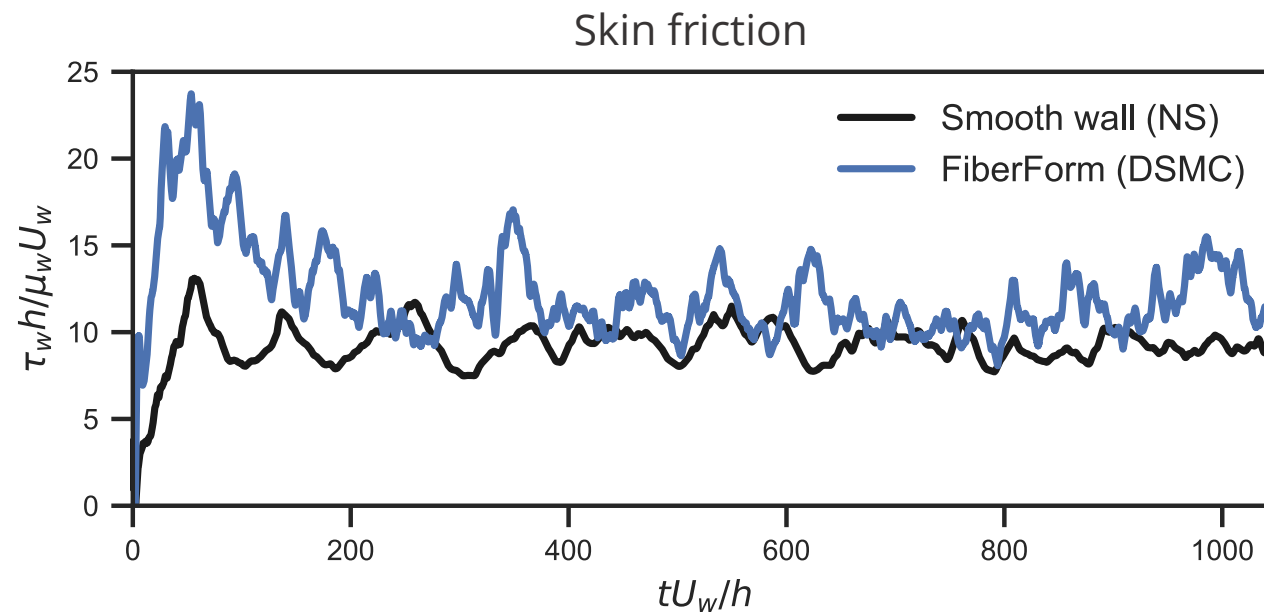


~20% mean and ~130% rms drag increase over smooth wall (NS) at same Re

Roughness and permeability can both increase drag [1] – difficult to disentangle the two causes

Substrate modifies turbulence across entire channel

Standard roughness models used in hypersonics aren't accurate for these kinds of permeable-wall flows



Improved roughness models are needed to account for permeability effects!

Substrate permeability

Intrinsic (Darcy) permeability (calculated with chfem_gpu [1]):

$$\mathbf{K}_0 \approx K_{y0} \begin{pmatrix} 1.77 & & \\ & 1 & \\ & & 1.82 \end{pmatrix},$$

$$K_{y0} = 5.13 \times 10^{-11} \text{ m}^2$$

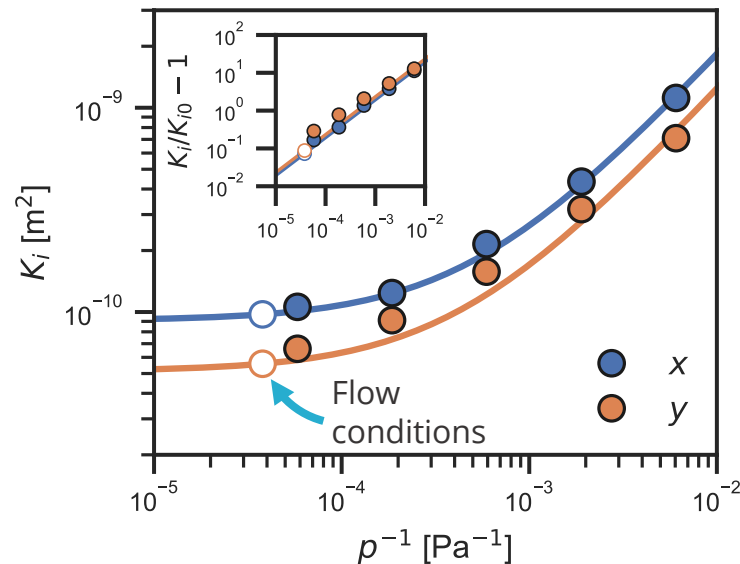
Klinkenberg [2] rarefaction correction:

$$\mathbf{K} = \mathbf{K}_0 \left[\mathbf{I} + p^{-1} \mathbf{b}(T, m, \mu) \right],$$

$$\mathbf{b}(T, m, \mu) = \frac{\mu}{\mu_{\text{ref}}} \sqrt{\frac{T}{T_{\text{ref}}}} \frac{m_{\text{ref}}}{m} \mathbf{b}_{\text{ref}}$$

Reference values from Borner et al. [3]

Quantity	Value
p	26.4 kPa
b_y	2.32 kPa
b_x	1.92 kPa
b_y / p	0.088
b_x / p	0.073
K_y	$\sim 6 \times 10^{-11} \text{ m}^2$
$K_x \approx K_z$	$\sim 1 \times 10^{-10} \text{ m}^2$



Circles: DSMC
Curves: Klinkenberg [3]

Rarefaction enhances permeability by ~10%

- [1] Lopes et al., CMS (2023)
[2] Klinkenberg (1941)
[3] Borner et al., IJHMT (2017)

Flow regime



Permeability has profound impact on overlying turbulence

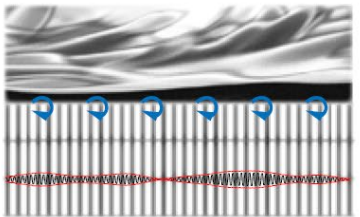
High permeability ($\sqrt{K^+} \gg 1$): canonical smooth-wall structures replaced by spanwise Kelvin-Helmholtz-like rollers [1]

Semi-empirical correlation for onset of K-H-like regime [2]:

$$\sqrt{K_{Br}^+} \approx \sqrt{K_y^+} \tanh^{1/2} \left(\frac{\sqrt{2K_x^+}}{9} \right) \gtrsim 0.5$$

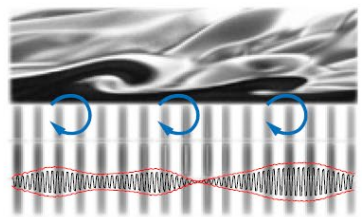
Increasing permeability

Smooth-wall-like regime



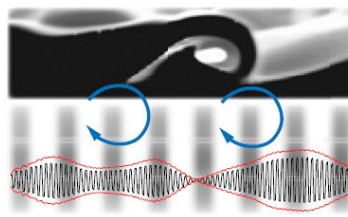
Effectively impermeable

K-H-like regime



Highly permeable

Mixing-layer regime



Canopy flow

[3]

Quantity	Value
τ_{avg}	293 Pa
ρ_s	0.407 kg/m ³
μ_0	2.858 x 10 ⁻⁵ Pa s
u_{TS}	26.8 m/s
$K_x \approx K_z$	$\sim 1 \times 10^{-10}$ m ²
K_y	$\sim 6 \times 10^{-11}$ m ²
$\sqrt{K_x^+} \approx \sqrt{K_z^+}$	~ 4
$\sqrt{K_y^+}$	~ 3
$\sqrt{K_{Br}^+}$	~ 2

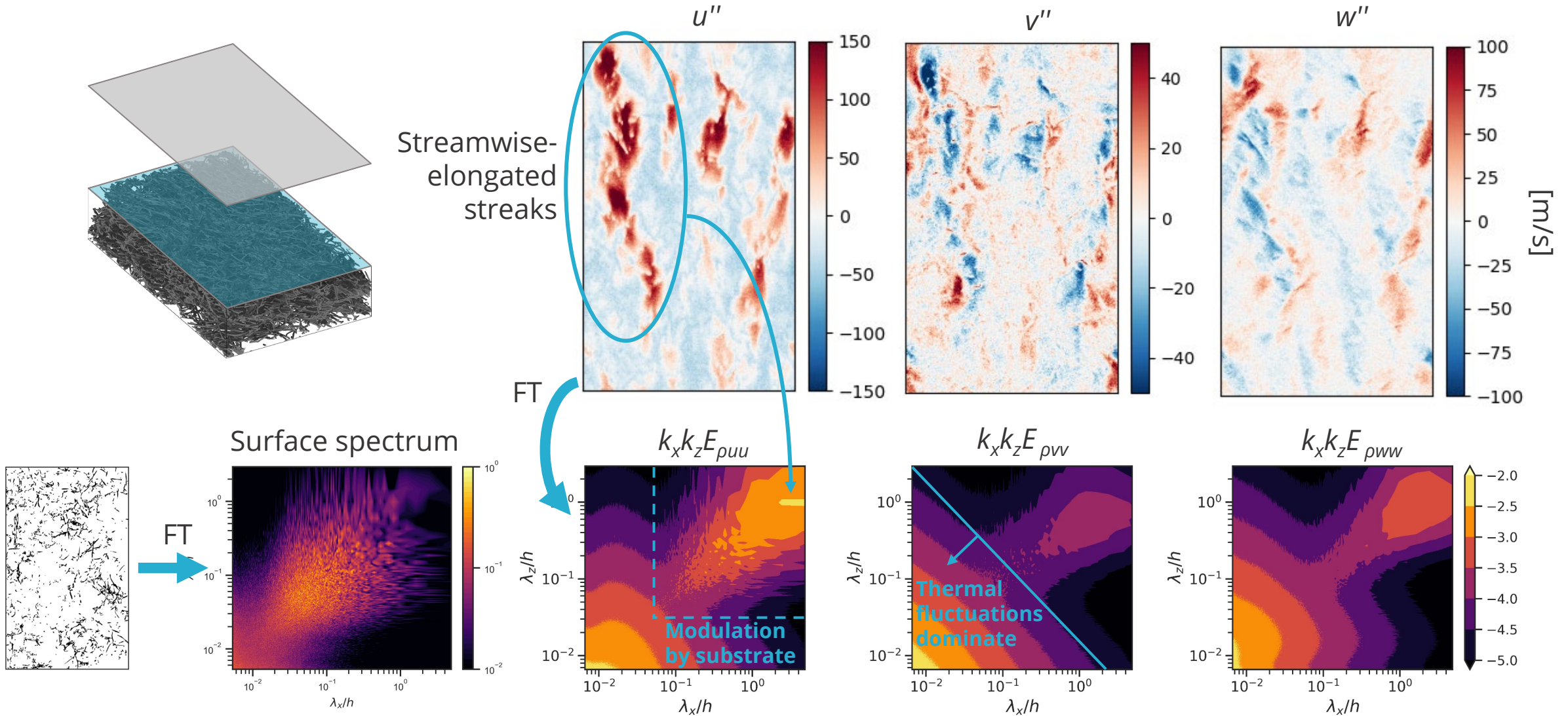
Based on K_{Br}^+ , expect to be in K-H-like regime.

[1] Breugem et al., JFM (2006)

[2] Gómez-de-Segura et al., FTC (2018)

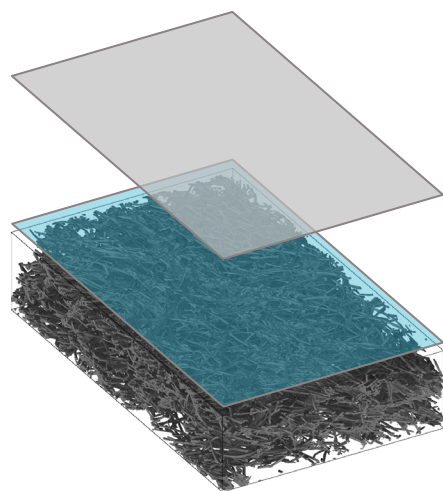
[3] Habibi Khorasani et al., JFM (2024)

Turbulence structures: substrate surface

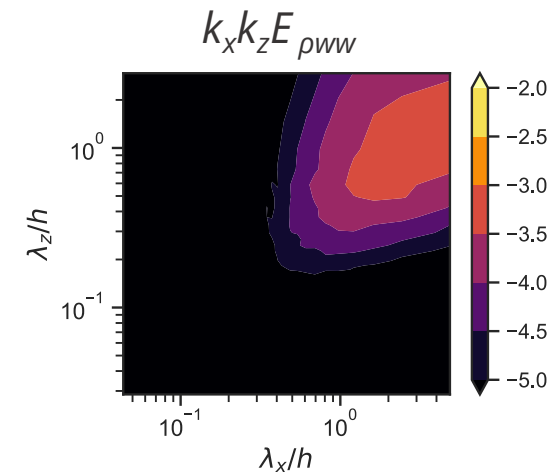
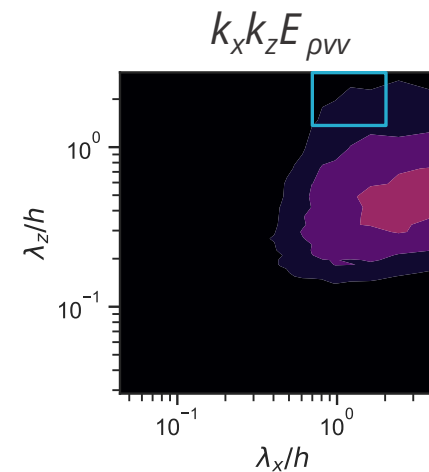
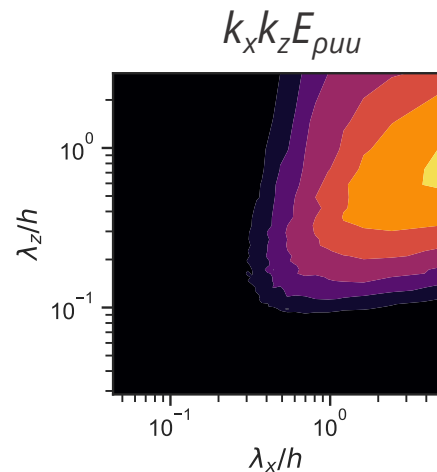


Smooth-wall-like structures modulated by substrate

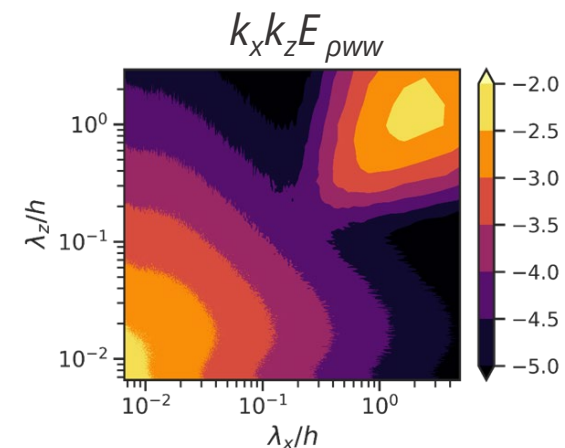
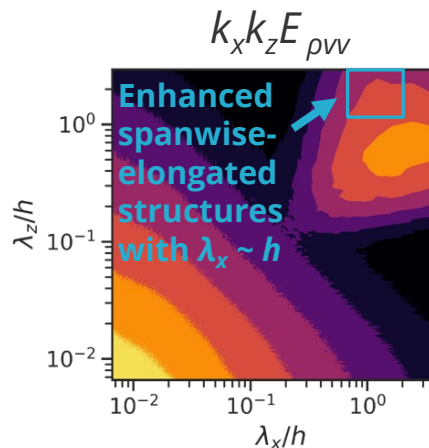
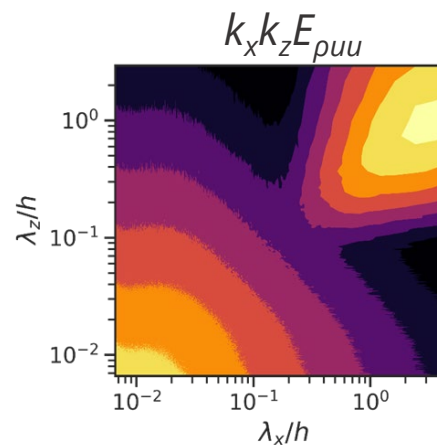
Turbulence structures: near-substrate ($y/h = -0.9$)



Smooth
wall (NS)



FiberForm
(DSMC)

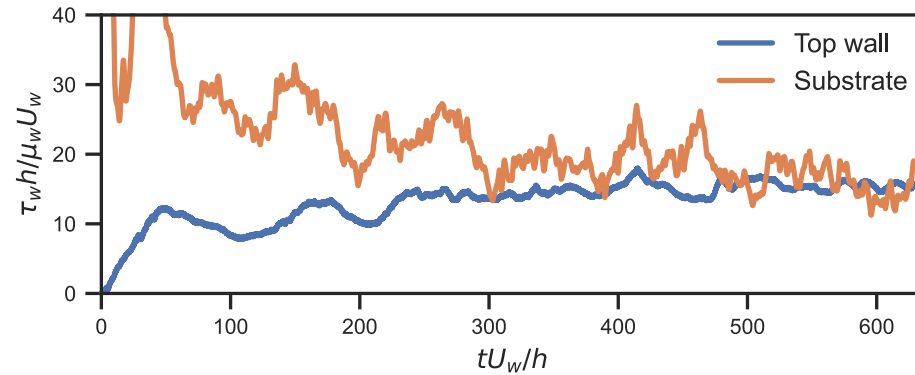


No clear evidence of K-H-like spanwise rollers, despite having $\sqrt{K_{Br}^+} \sim 2$

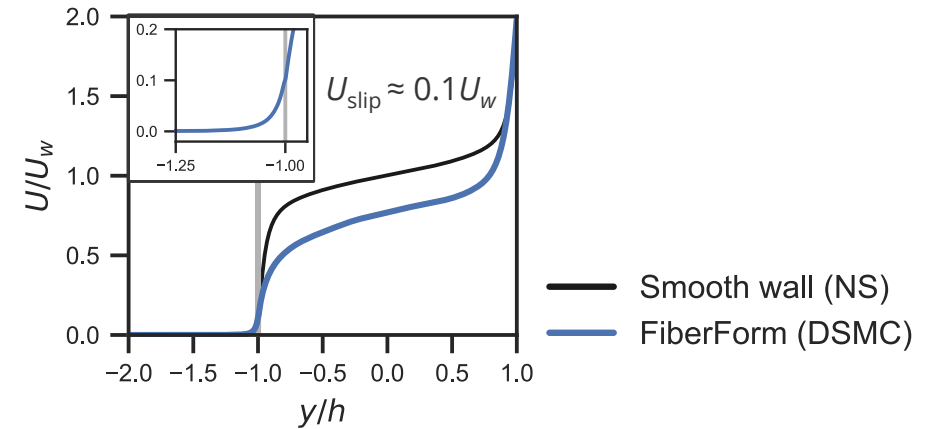
Higher Mach number: $Ma_0 = 3$ ($Re_0 = 5600$)



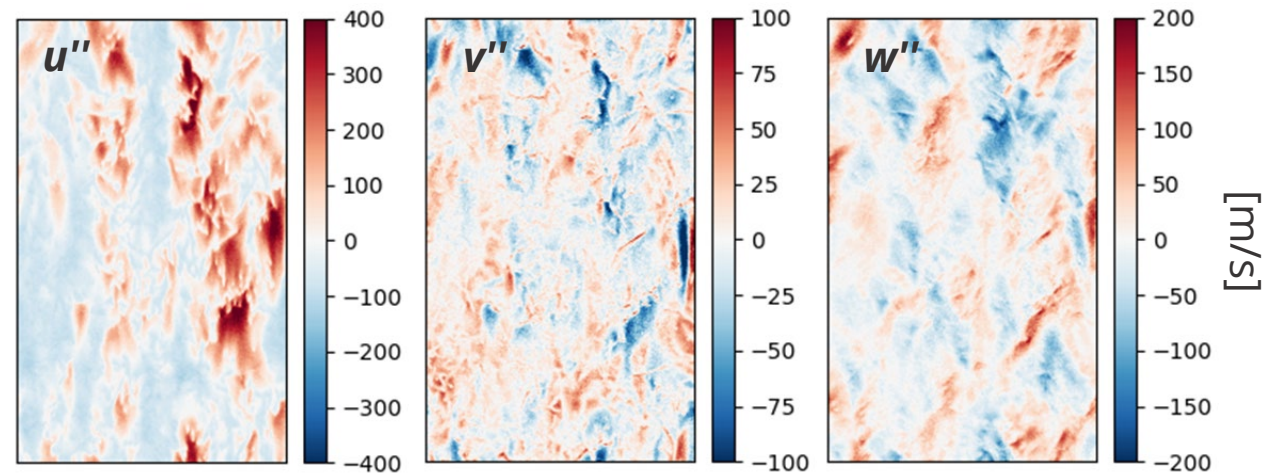
Skin friction shows slow approach to steady-state



Slip velocity appears to scale with U_w



Near-surface turbulence structures still dominated by streamwise streaks



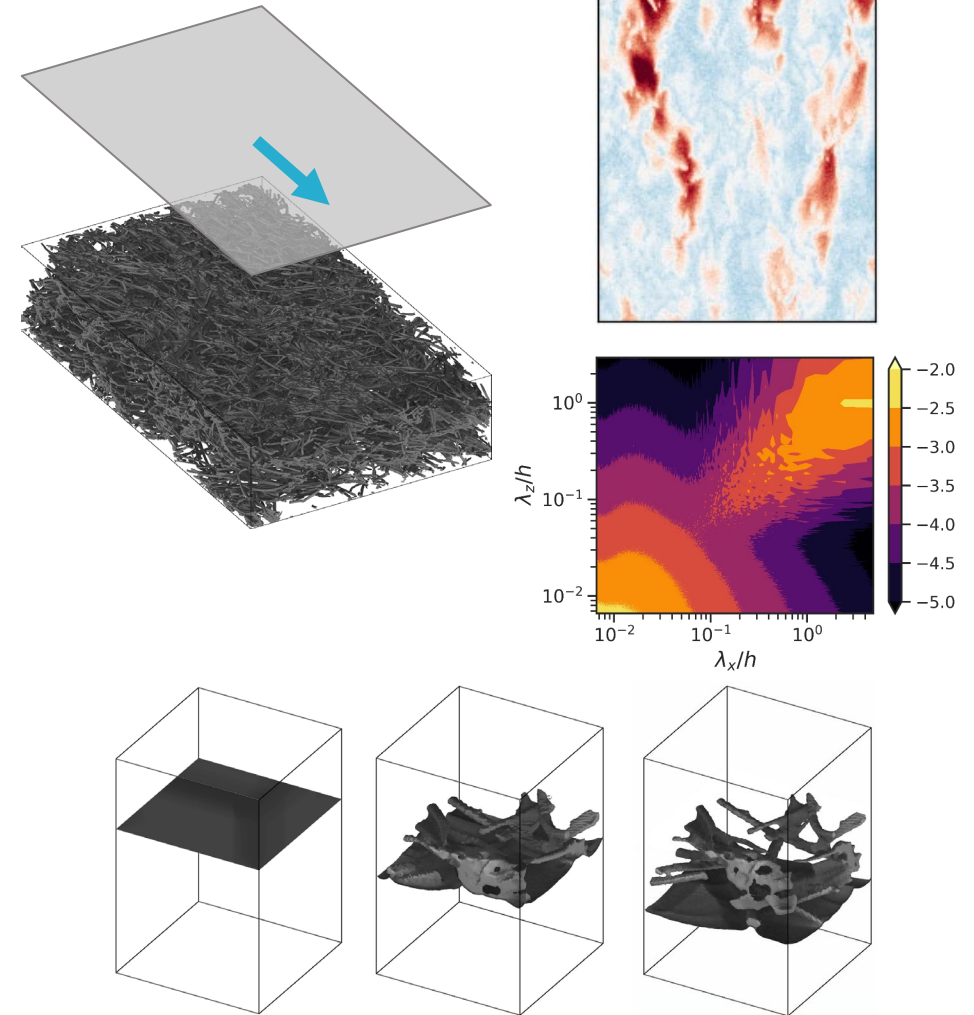
Summary

Investigation of turbulent flow over 3D scan of a real TPS material using DSMC

- Simulations fully resolve pore-scale flow through complex FiberForm substrate
- Rarefaction enhances substrate permeability by ~10%
- No clear evidence of K-H-like rollers, despite having $\sqrt{K_{Br}^+} \sim 2$. Possible explanations:
 - Streamwise rolls in turbulent Couette flow suppress them [1]
 - Domain not wide enough to clearly distinguish from other structures

Future work:

- Higher-speed flows ($Ma_0 = 5$, $Re_0 = 9300$ simulation underway)
- Ablation (New capabilities recently implemented in SPARTA)



SPARTA ablation simulation by A. Hong

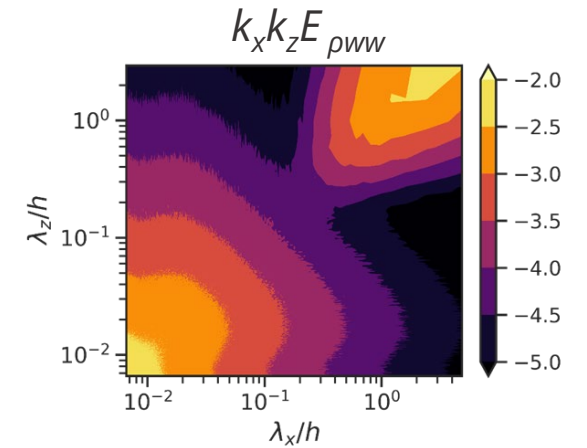
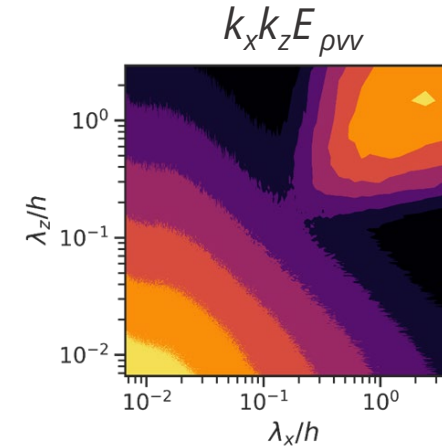
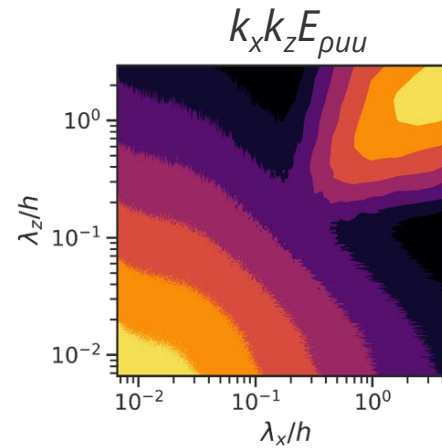
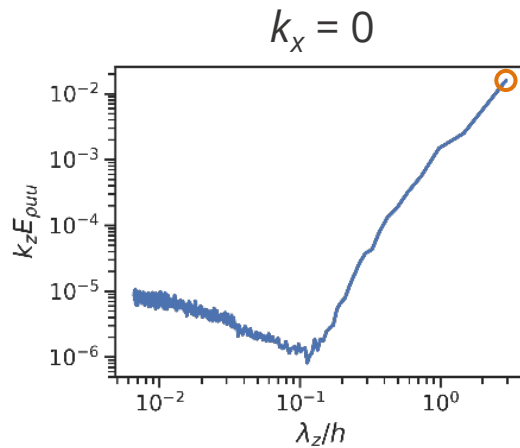
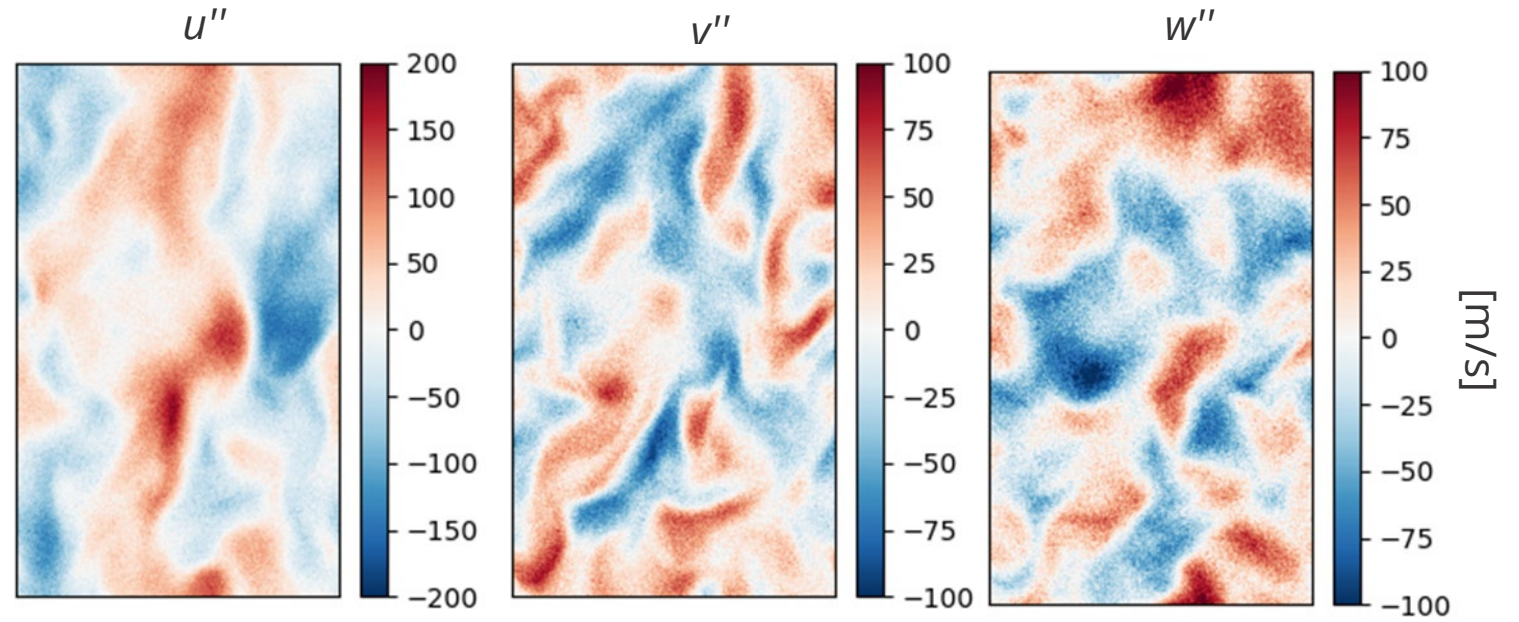
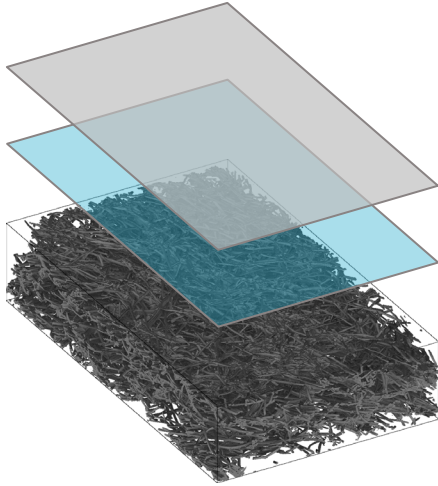
DSMC can be a valuable tool for simulating turbulent flows in conditions that are challenging for conventional CFD!



Backup

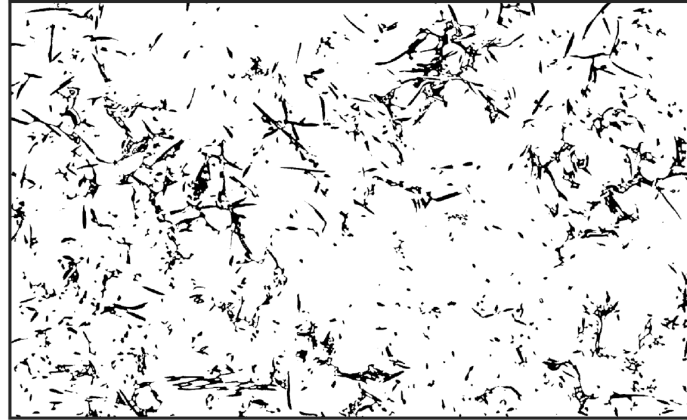


Turbulence structures: channel center

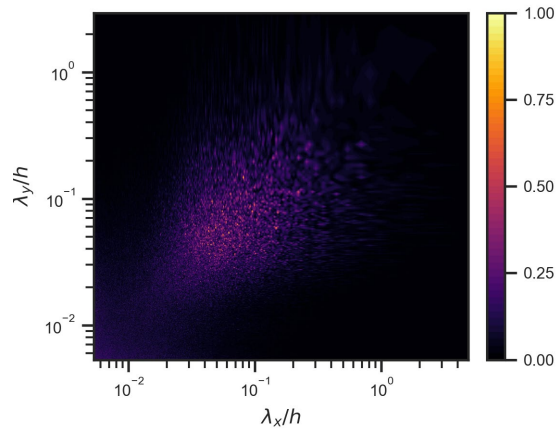


Streamwise rolls dominate far from the substrate

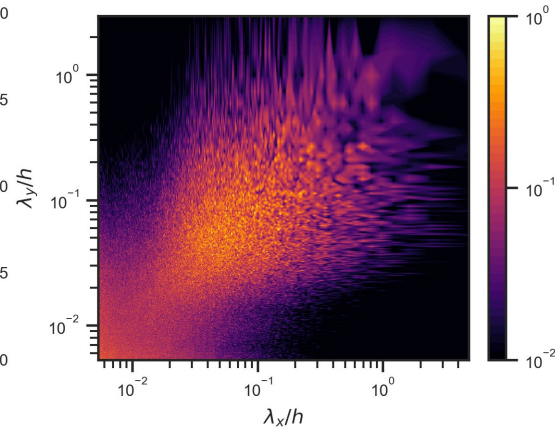
Substrate properties



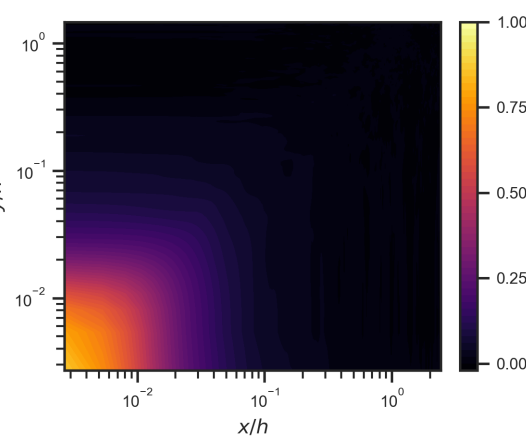
Spectrum



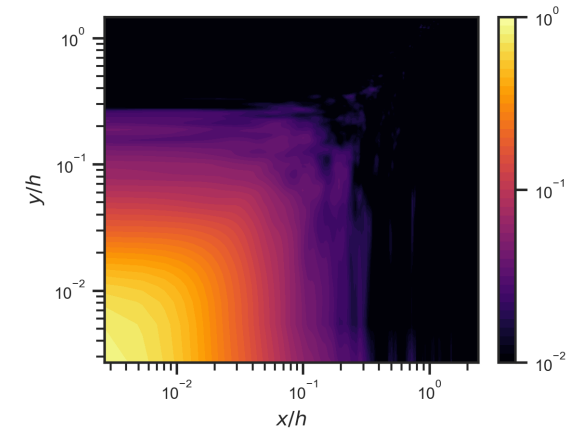
Spectrum (log scale)



Autocorrelation



Autocorrelation (log scale)



Dimensional quantity	Value
h	$5.002 \times 10^{-4} \text{ m}$
T_w	273.15 K
U_w	461.85 m/s
a_w	307.9 m/s
μ_w	$2.858 \times 10^{-5} \text{ Pa s}$
ρ_0	0.345 kg/m^3
ρ_w	0.449 kg/m^3
ρ_s	0.407 kg/m^3
λ_0	$4.35 \times 10^{-7} \text{ m}$
λ_w	$3.23 \times 10^{-7} \text{ m}$
λ_s	$3.69 \times 10^{-7} \text{ m}$
$\tau_{w,\text{avg}}$	293 Pa
$u_{\tau,w}$	25.5 m/s
$u_{\tau,s}$	26.8 m/s
$K_x \approx K_z$	$9.9 \times 10^{-11} \text{ m}^2$
K_y	$5.6 \times 10^{-11} \text{ m}^2$

Nondimensional quantity	Value
Re_0	2790
$\text{Re}_{\tau,w}$	201
$\text{Re}_{\tau,s}$	182
Ma_0	1.5
Kn_0	8.7×10^{-4}
Kn_w	6.7×10^{-4}
Kn_s	7.4×10^{-4}
$\text{Kn}_{\tau,w}$	0.13
$\text{Kn}_{\tau,s}$	0.13
K_x/K_y	1.75
$\sqrt{K_x^+} = \sqrt{K_x^+}$	3.8
$\sqrt{K_y^+}$	2.9
$\sqrt{K_{\text{Br}}^+}$	2.1