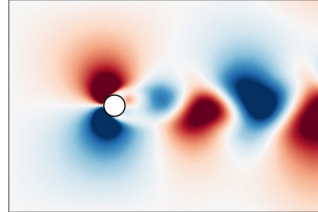
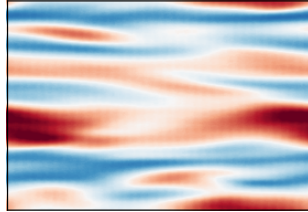
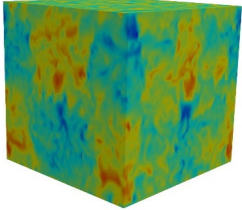
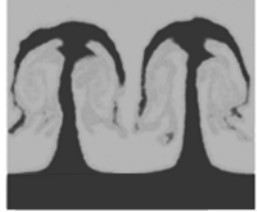




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Molecular-level simulations of turbulent Couette flow over a thermal-protection- system material



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Flow over thermal-protection-system materials



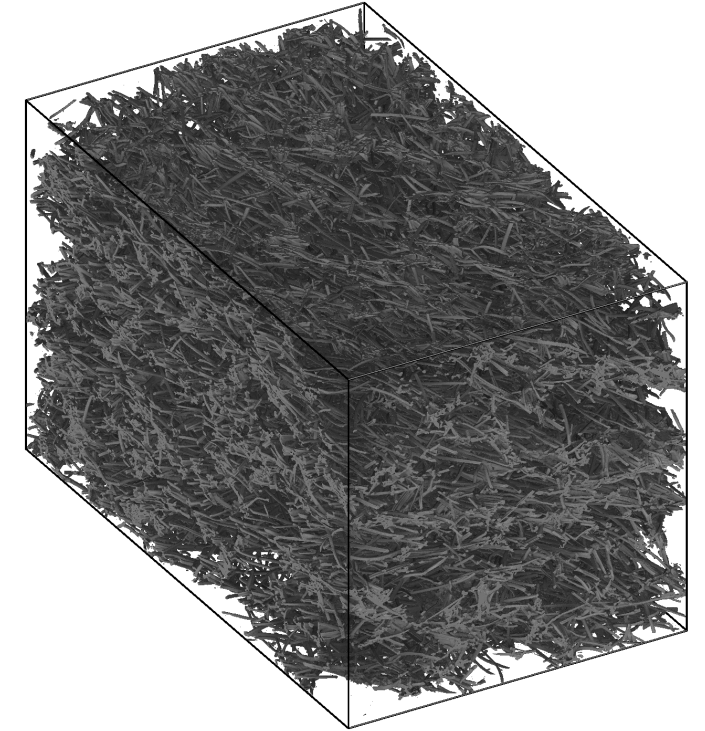
Thermal-protection-system (TPS) materials on reentry vehicles may be:

- Rough
 - Permeable
- Affects aerothermal loading and may compromise vehicle performance

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

- Noncontinuum effects may be significant within the substrate (Klinkenberg effect)
- Substrate geometry can be difficult to mesh, even with immersed boundary methods

Direct Simulation Monte Carlo (DSMC) is well-suited for simulating flow over TPS materials!



3D scan of FiberForm

Goal: Assess roughness and permeability effects in compressible turbulent flow over TPS materials with DSMC

Direct simulation Monte Carlo (DSMC)



DSMC is the dominant method for molecular gas dynamics [1]

No PDEs solved - tracks very large numbers ($\sim 10^{12}$) of particles, each representing many actual molecules

- Move ballistically, collide & reflect stochastically
- Flow quantities from averages over molecules in each cell

Inherently includes physics usually not in traditional CFD

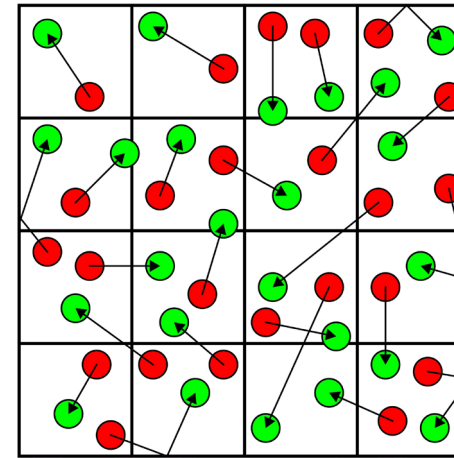
- Thermal and chemical nonequilibrium
- Pressure and heat-flux tensor anisotropy
- Thermal fluctuations

Simulates gas flows very accurately

- Solutions converge to solutions of the Boltzmann Equation [2]
- Reproduces Chapman-Enskog distribution [3]

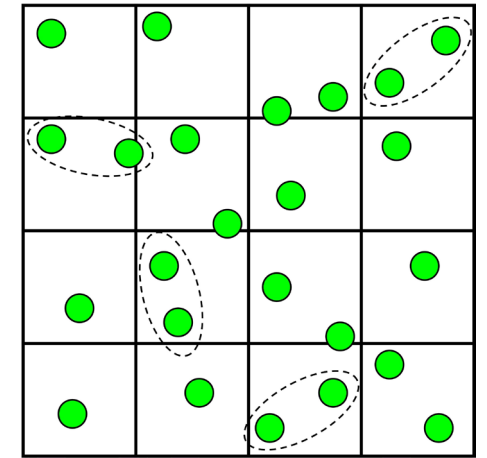
Computational and algorithmic advances have brought turbulent flows within reach of DSMC!

move



$$\frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i$$

collide



$$\frac{d(m_i \mathbf{v}_i)}{dt} = \mathbf{F}(\mathbf{x}_i) + \mathbf{C}(\mathbf{v}_i)$$

[1] Bird, Clarendon Press (1994)
 [2] Wagner, J. Stat. Phys. (1992)
 [3] Gallis et al., Phys. Rev. E (2004)

SPARTA: An exascale DSMC code

SPARTA: Stochastic PARallel Rarefied-gas Time-accurate Analyzer

Implementation is similar to Molecular Dynamics

- Single-processor to massively-parallel platforms
- Load balancing, in-situ visualization, on-the-fly FFTs, adaptive grid

Developed with next-generation architectures in mind

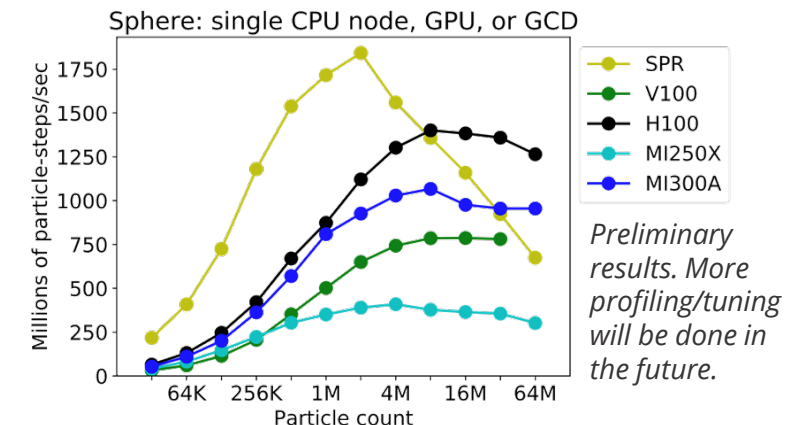
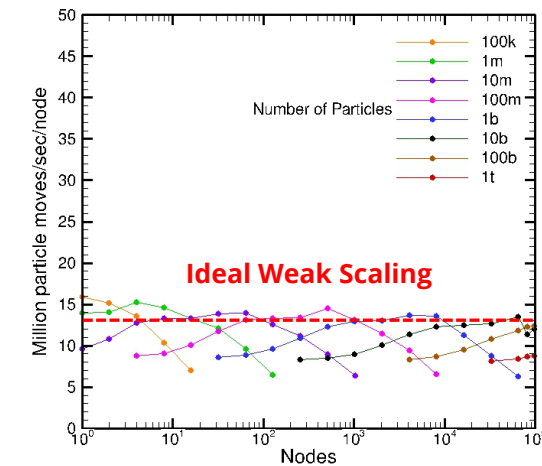
- Write application kernels only once
- Efficient on many platforms: GPU, manycore, heterogeneous, ...

Complex geometries are easily treated

- Domain can be 2D, axisymmetric, 3D
- Gas molecules use hierarchical Cartesian grid
- Body surfaces represented by triangular elements which cut gas grid cells

Open-source code available: <http://sparta.sandia.gov>

- 10,000+ downloads, 100+ verified users worldwide
- Collaborators: ORNL, LANL, ANL, LBNL, NASA, ESA, Purdue, UIUC



FiberForm substrate



FiberForm is the substrate for NASA's PICA TPS

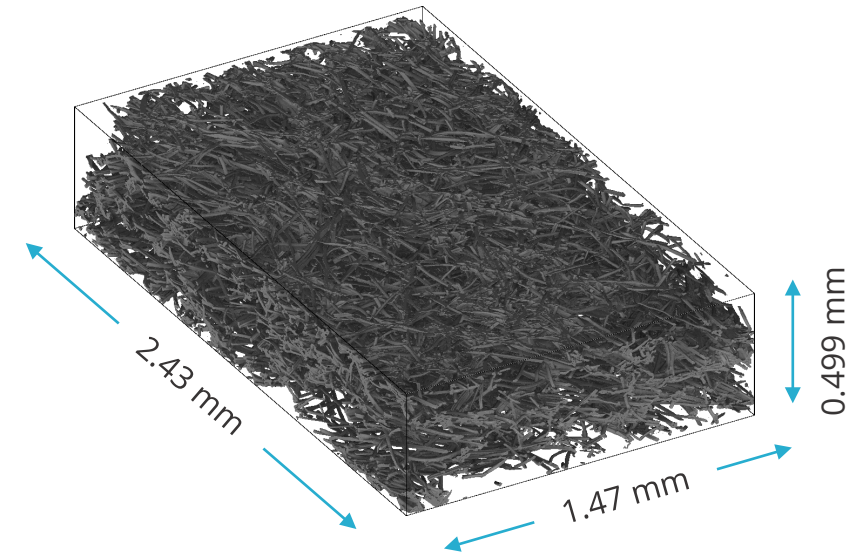
- Porosity: 0.86
- Fiber diameter: $\sim 10\ \mu\text{m}$
- Mean pore diameter: $\sim 50\ \mu\text{m}$

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)

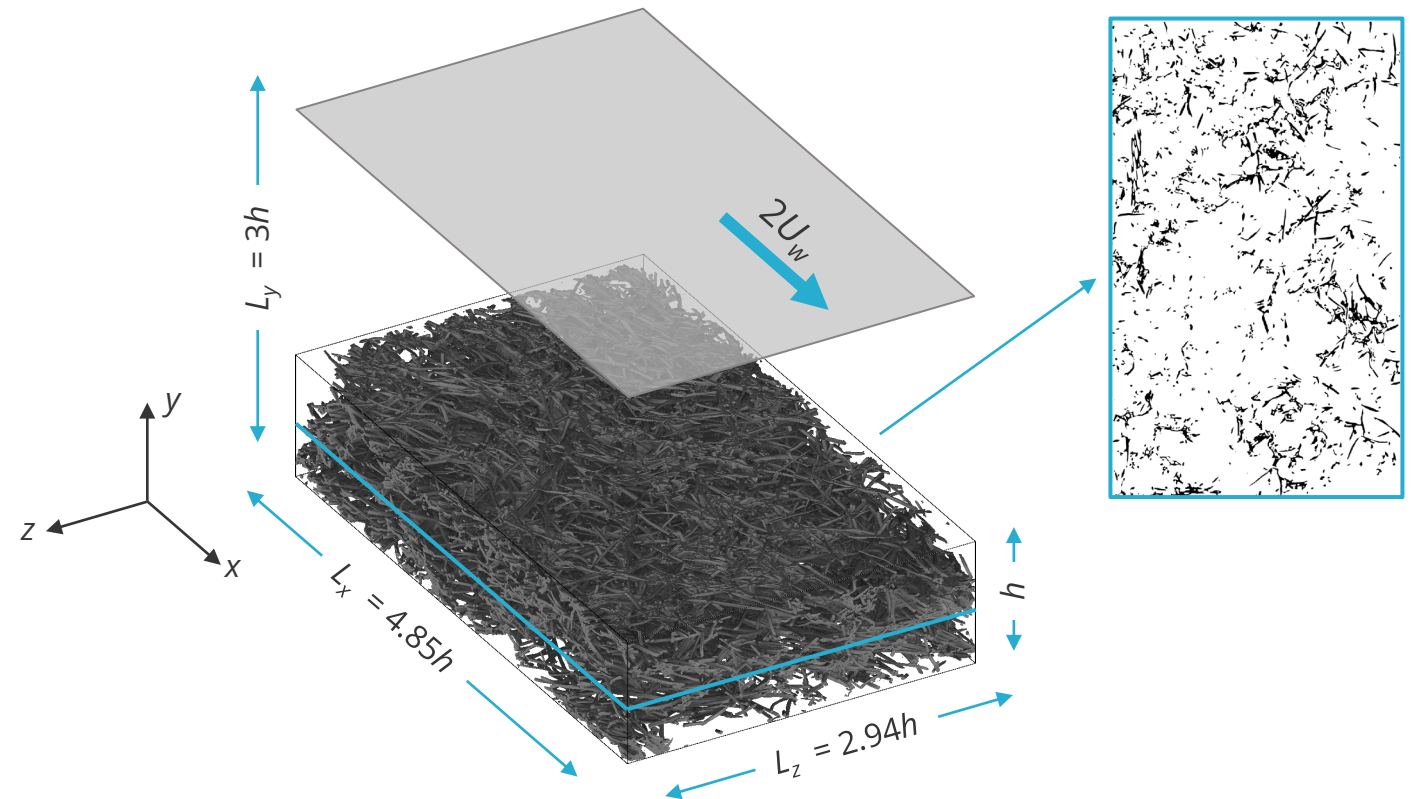


Enables pore-scale-resolved turbulence simulations over a real material sample

Turbulent Couette flow over TPS material



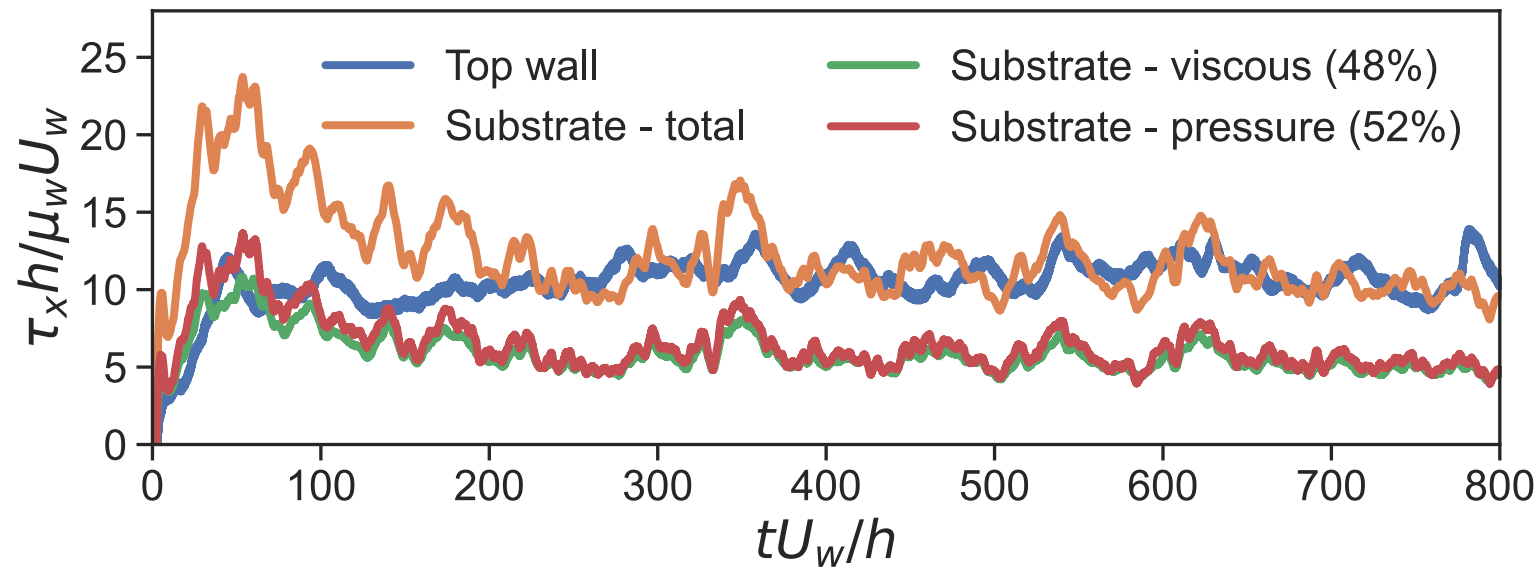
- Length scale: $h = 500 \mu\text{m}$
- Cell size: $1.65 \mu\text{m}$
- Total cells: 1.19×10^9
- Total particles: 34×10^9
- Avg. particles per cell: 29
- Time step: 9.12 ps
- Monatomic gas: $\gamma = 5/3$
- Molecular mass: $6.63 \times 10^{-26} \text{ kg}$
- Walls: diffuse reflections, $\alpha = 1$, $T_0 = 273.15 \text{ K}$
- Periodic in x and z directions



Ma_0	Re_0	Kn_0
1.5	2790	8.7×10^{-4}

$$Ma_0 = U_w/a_0 \quad Re_0 = \rho_0 U_w h / \mu_w \quad Kn_0 = \lambda_0/h$$

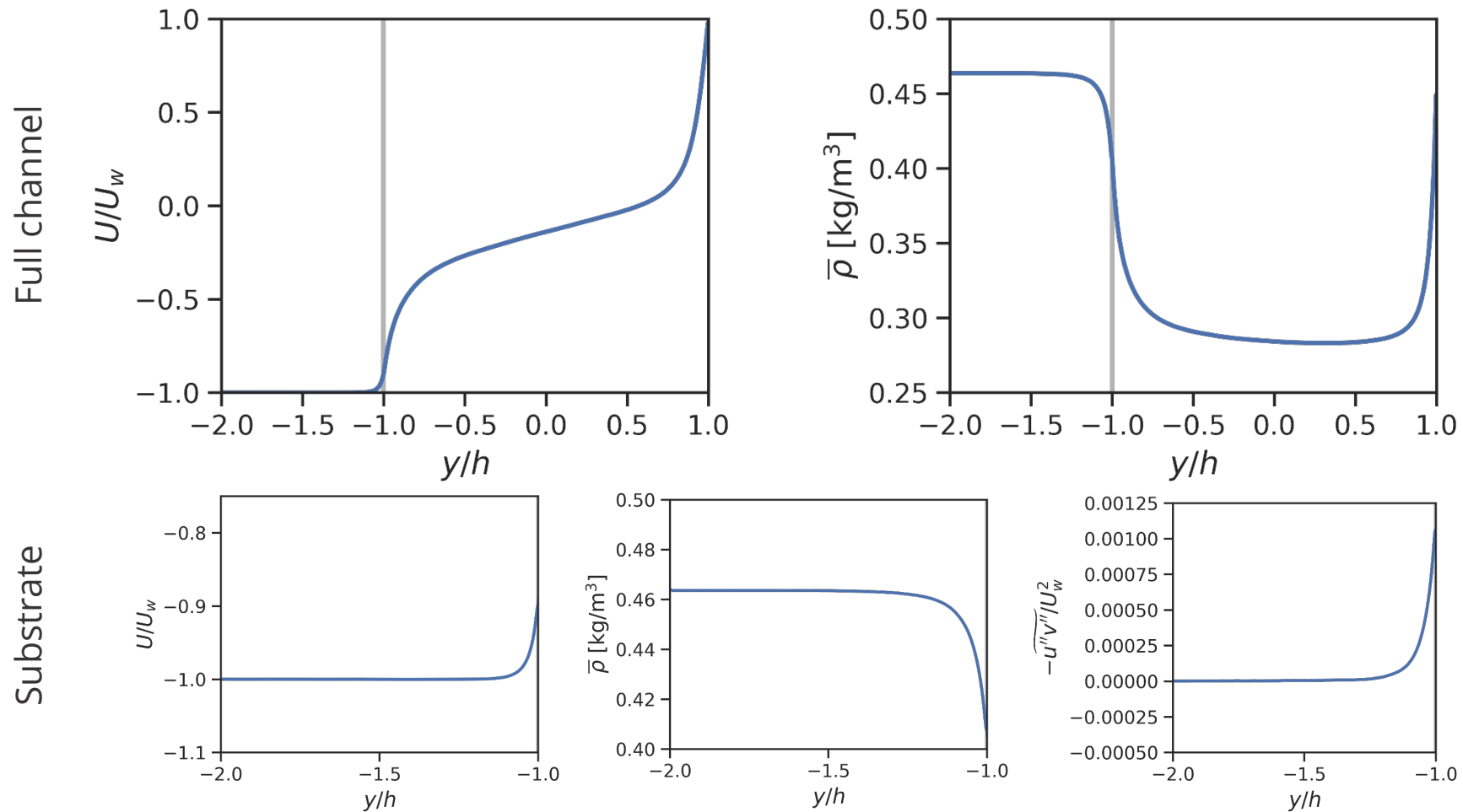
Skin friction



$$\tau_{\text{avg}} h / \mu_w U_w = 11.1 \quad (tU_w/h \geq 250)$$

~20% drag increase over smooth wall at same Re

Substrate: viscous drag $\approx$ pressure drag $\rightarrow$ transitionally rough regime



Substantial interface slip velocity: $U_{\text{slip}}/U_w = 0.11$, $U_{\text{slip}}^+ = 1.9$

Flow only penetrates ~25% of substrate depth $\rightarrow$ infinite-depth regime

Substrate permeability



Intrinsic (Darcy) permeability (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:

$$K = K_0 \left(1 + \frac{b(T, m, \mu)}{p} \right);$$

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

(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	5.6×10^{-11}
$K_x \approx K_z$	9.9×10^{-11}

Rarefaction enhances permeability by ~10%

[1] Lopes et al., CMS (2023)

[2] Klinkenberg (1941)

[3] Borner et al., IJHMT (2017)

Flow regime assessment



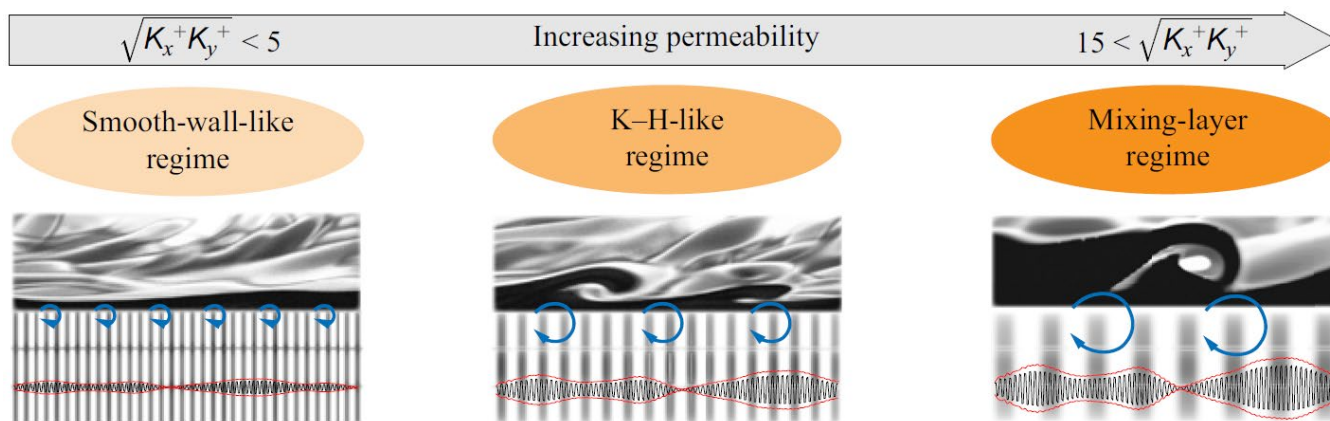
Permeability has profound impact on overlying turbulence

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

Semi-empirical correlation for K-H roller onset [2]:

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

$$\sqrt{K_{Br}^+} > 0.4 - 0.6$$



Nondimensional quantity	Value
$\tau_{w,avg}$	293 Pa
ρ_s	0.407 kg/m ³
μ_w	2.858 x 10 ⁻⁵ Pa s
$u_{t,s}$	26.8 m/s
$K_x \approx K_z$	9.9 x 10 ⁻¹¹ m ²
K_y	5.6 x 10 ⁻¹¹ m ²
$\sqrt{K_x^+} \approx \sqrt{K_z^+}$	3.8
$\sqrt{K_y^+}$	2.9
$\sqrt{K_{Br}^+}$	2.1

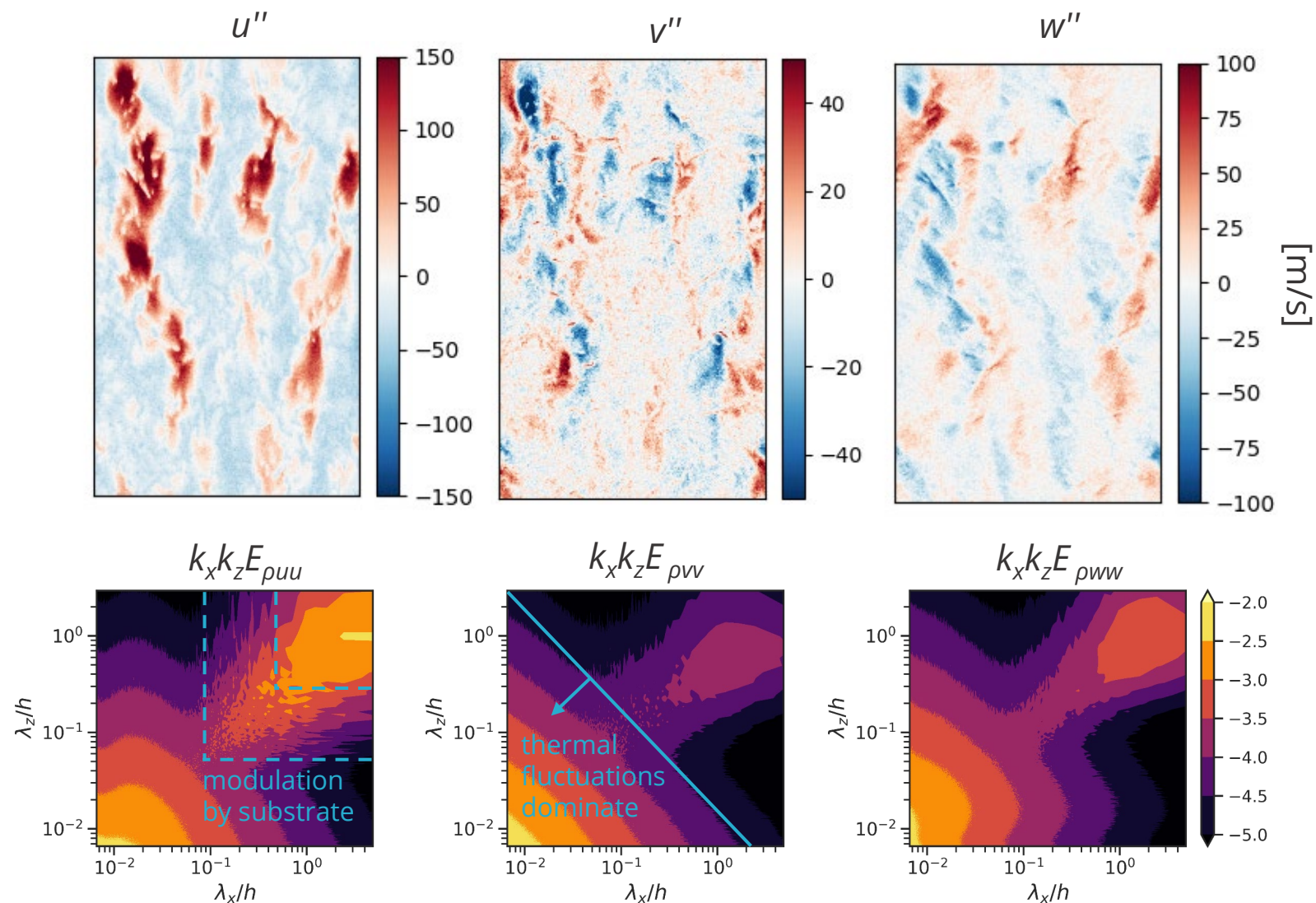
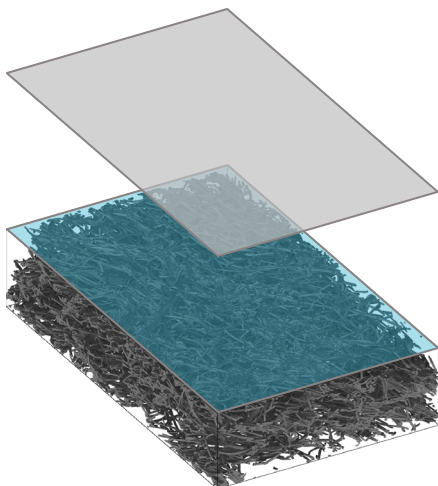
Based on K_{Br}^+ , expect to be in K-H-like regime.

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

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

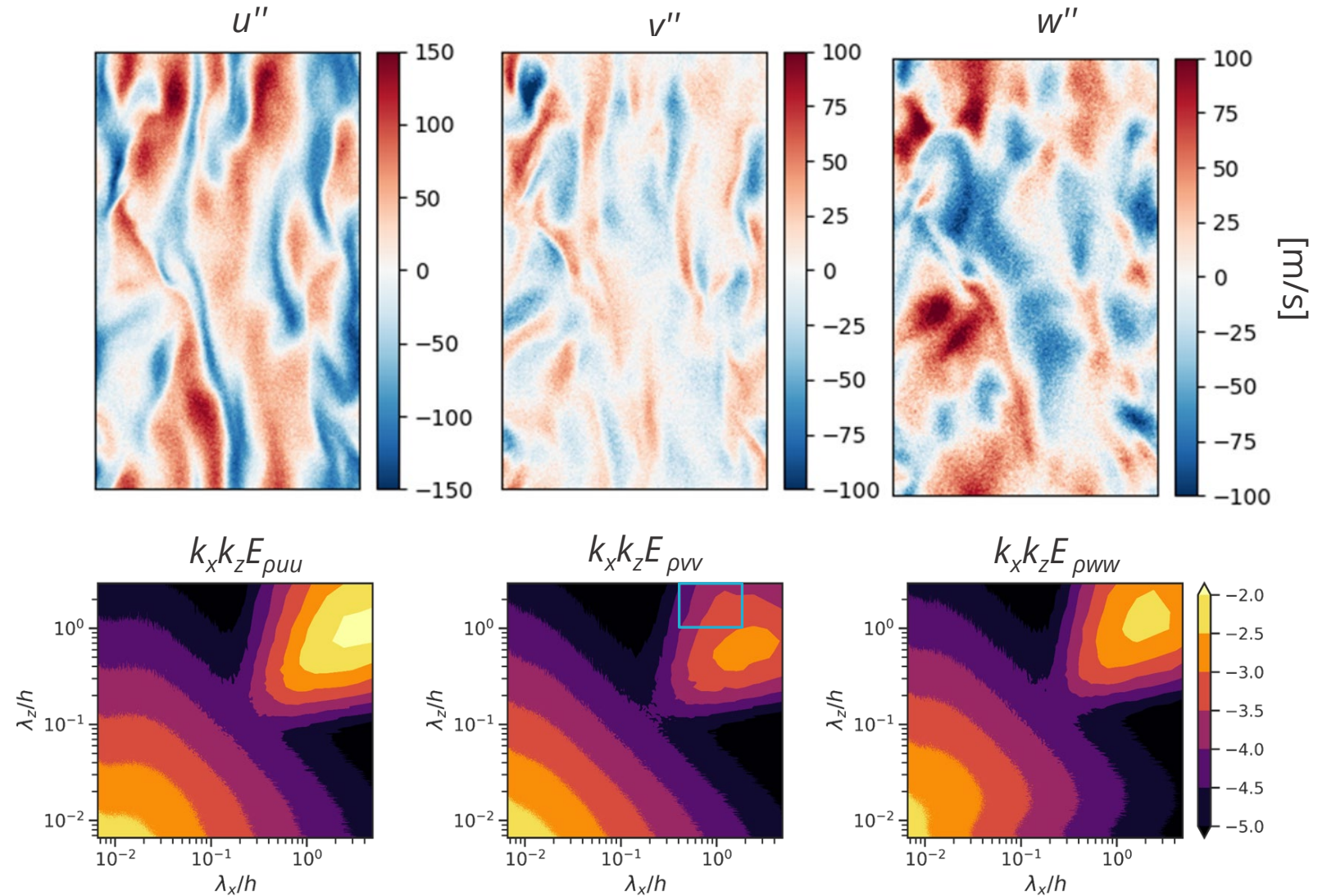
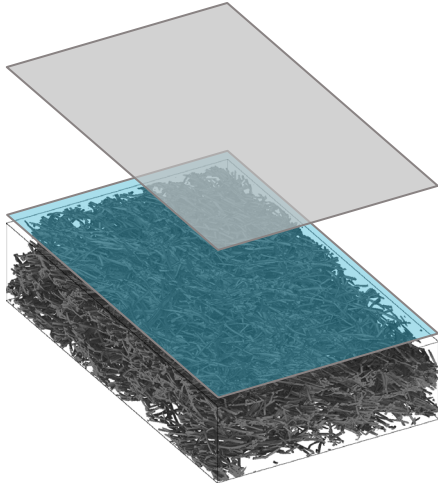
[3] Khorasani et al., JFM (2024)

Structures: substrate surface



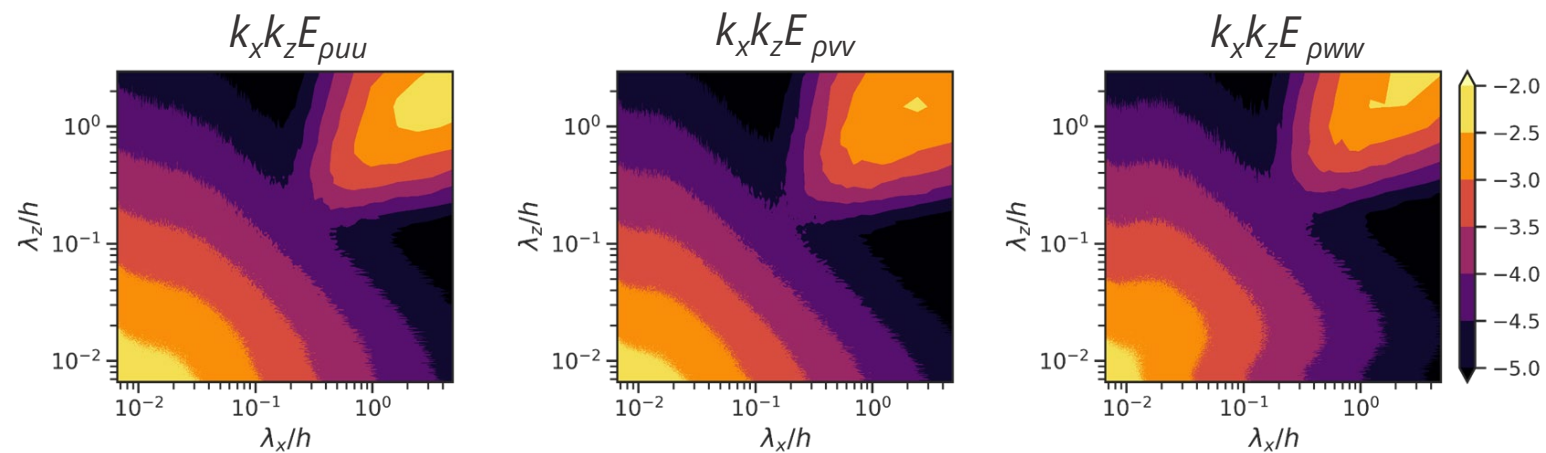
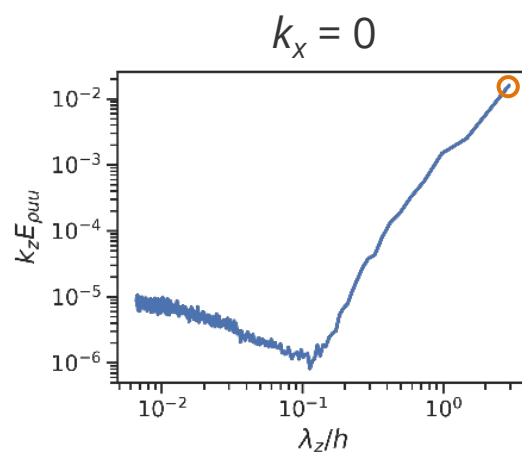
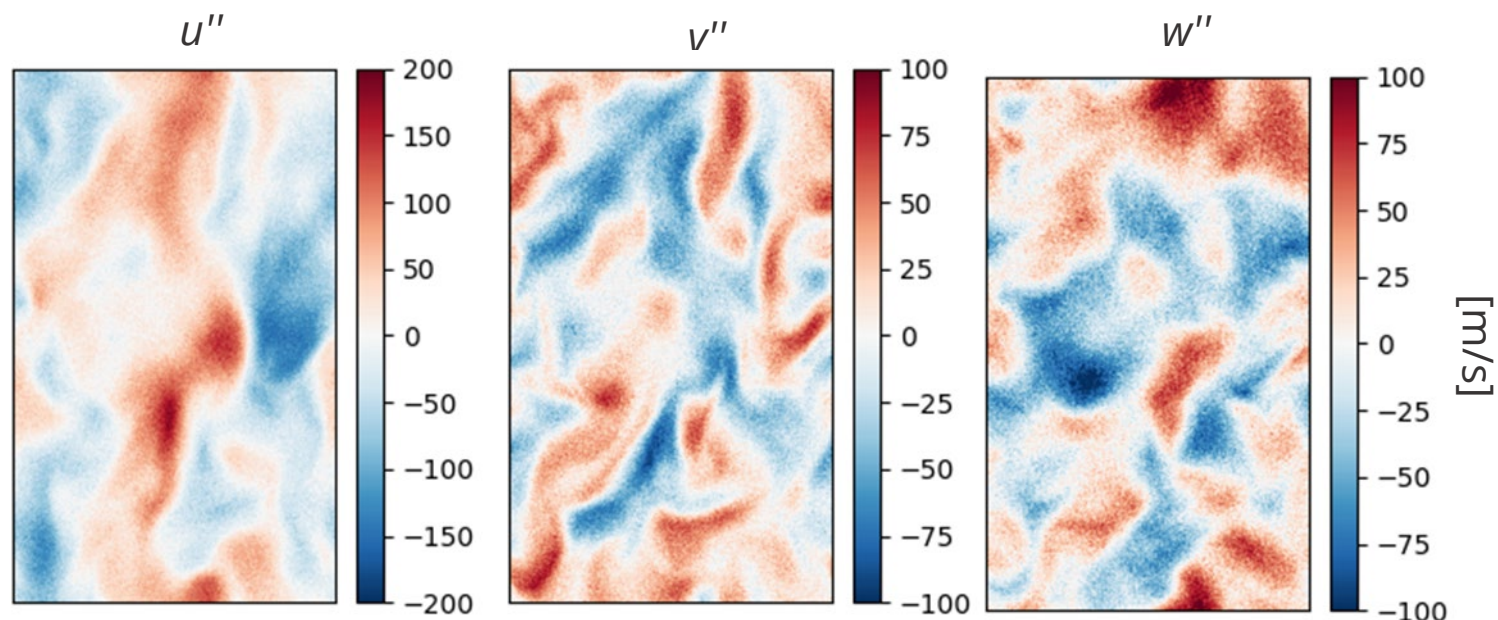
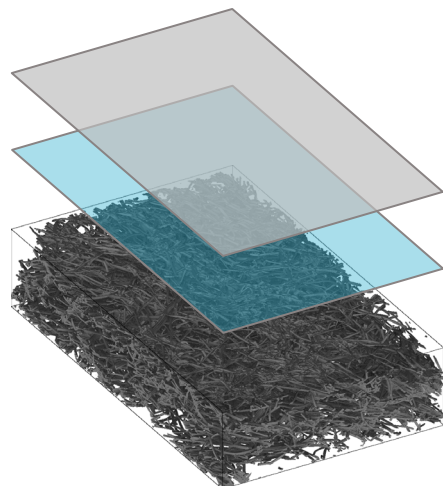
Smooth-wall-like structures modulated by substrate

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



No clear evidence of K-H-like spanwise rollers

Structures: channel center



Streamwise rolls dominate far from the substrate

Summary

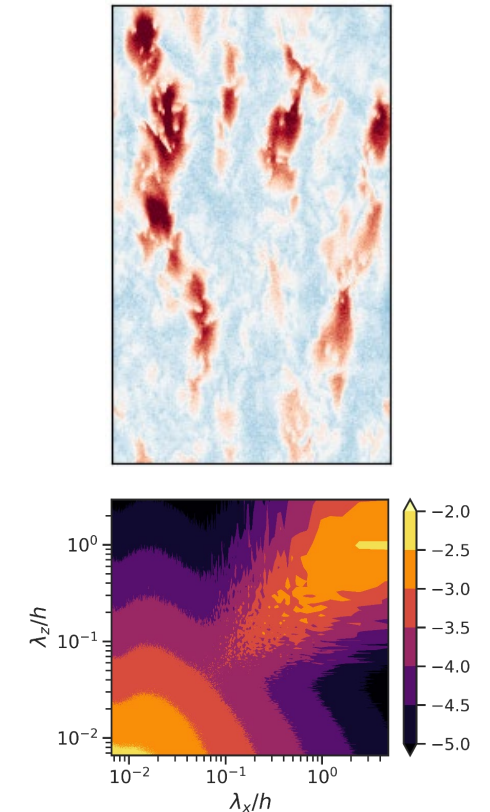
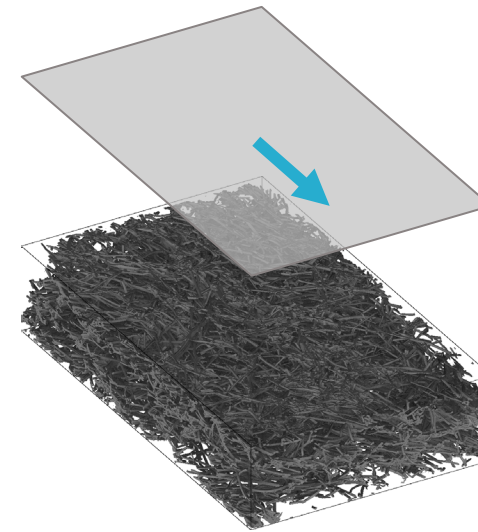


Preliminary investigation of turbulent flow over 3D scan of a real TPS material using DSMC

- Simulations fully resolve pore-scale flow through complex FiberForm substrate
- Modest ($\sim 10\%$) permeability enhancement by rarefaction
- Viscous and pressure drag on substrate both significant
- Substantial interface slip velocity; flow penetrates $\sim 25\%$ of substrate depth
- No evidence of K-H-like rollers, despite relatively large value of K_{Br}^+ . Possible explanations:
 - Streamwise rolls in turbulent Couette flow suppress them
 - Domain not wide enough to clearly delineate from other structures

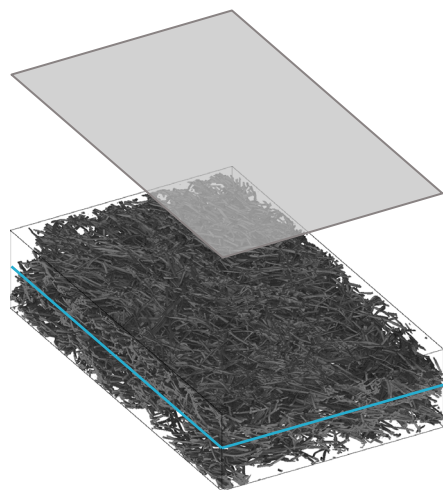
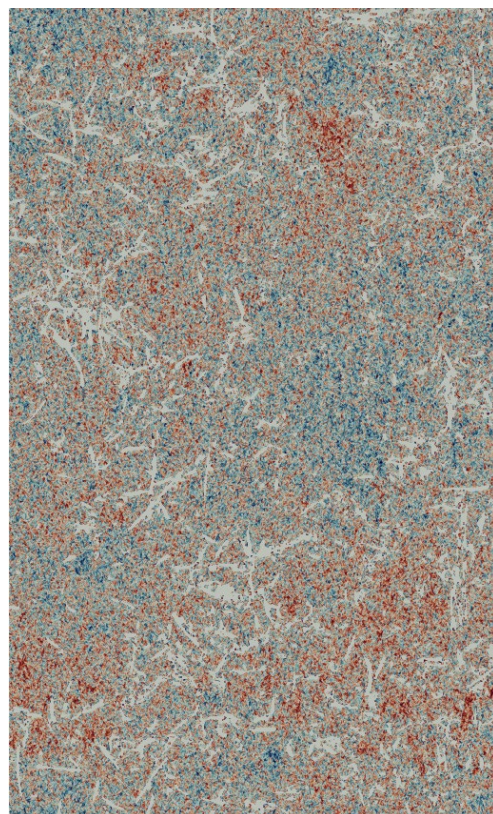
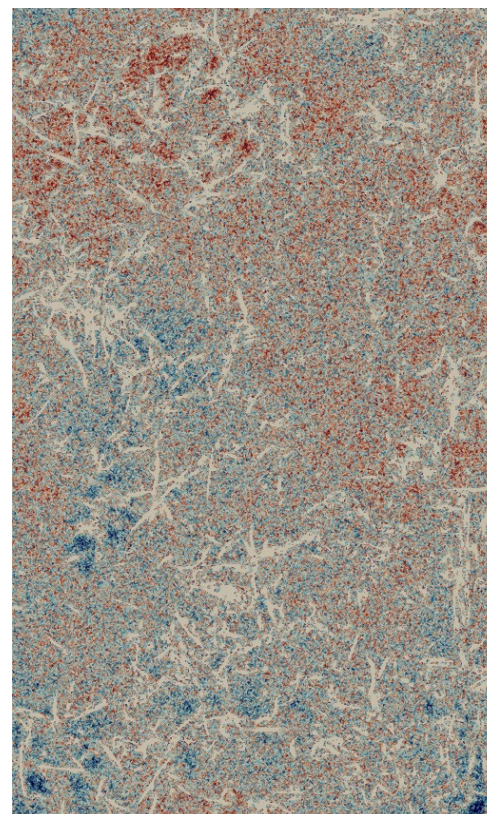
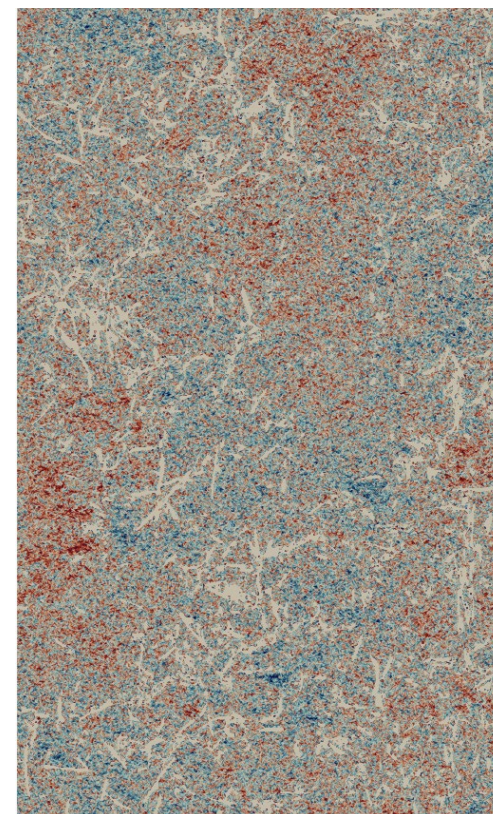
Future work:

- Higher Mach numbers ($Ma = 5$ simulation underway)
- Ablation (New capabilities recently implemented in SPARTA)



DSMC can be a valuable tool for simulating turbulent flows over surfaces and in conditions that are challenging for standard CFD!

Structures: mid-substrate

 u  v  w 

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