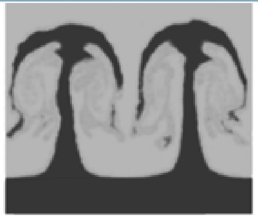
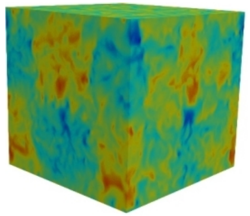
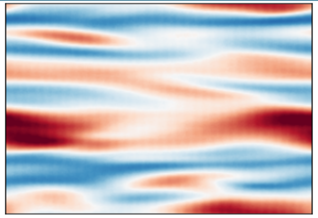
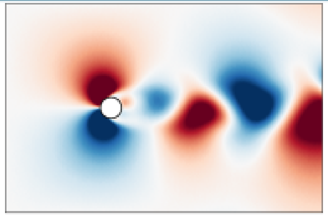
SAND2024-08837C

Molecular-level simulations of turbulent Couette flow over rough surfaces

Ryan M. McMullen, Timothy P. Koehler, Michael A. Gallis

33rd International Symposium on Rarefied Gas Dynamics (RGD33)

Göttingen, Germany

16 July, 2024

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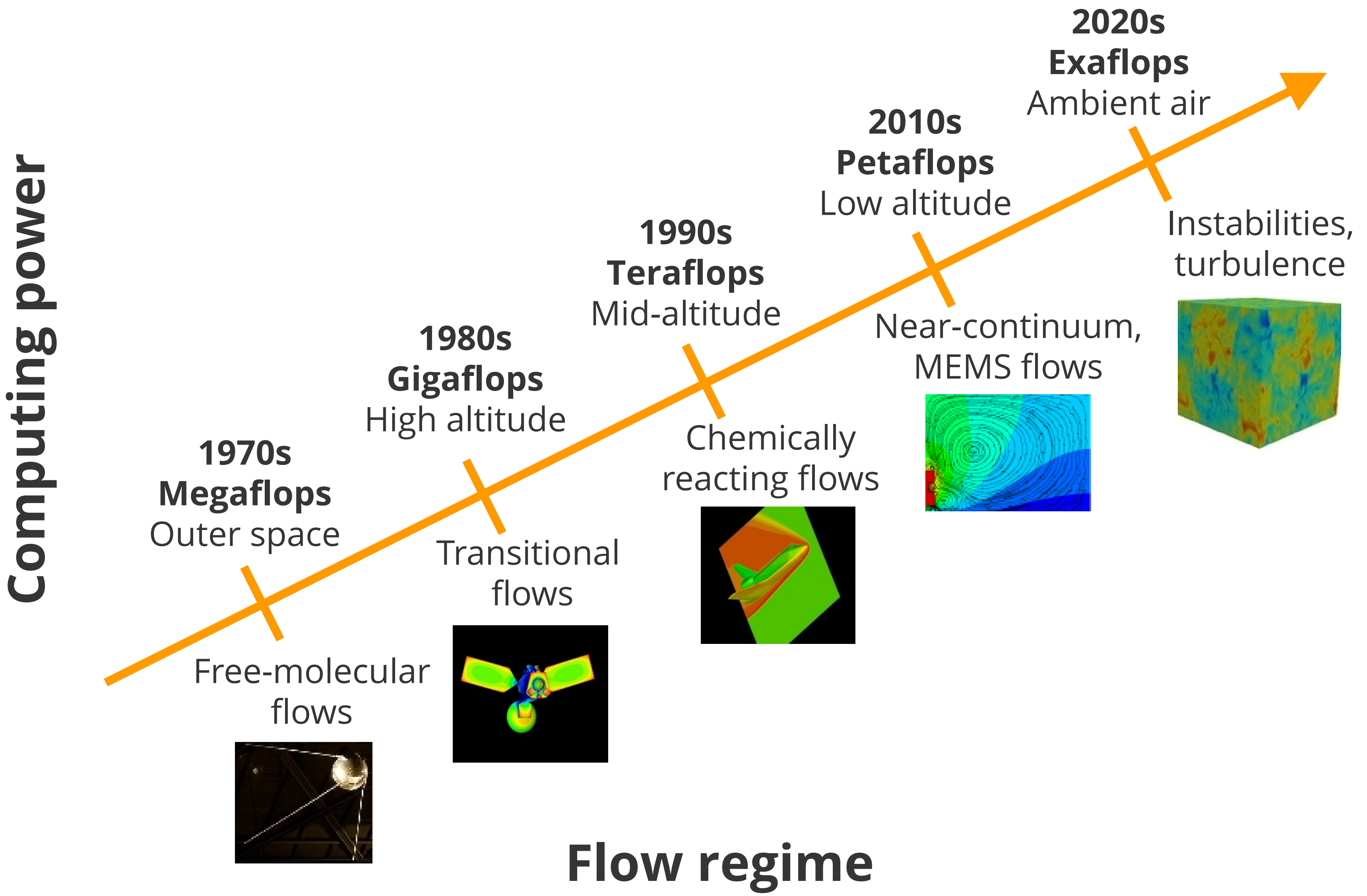
Molecular gas dynamics: from free-molecular flow to turbulence in 50 years



Direct simulation Monte Carlo (DSMC)

DSMC is the dominant method for MGD [1]

No PDEs solved - tracks very large numbers (~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

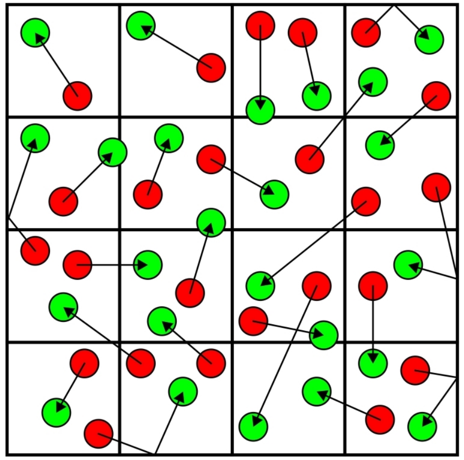
- Thermal and chemical nonequilibrium
- Pressure and heat-flux tensor anisotropy
- Thermal fluctuations

Simulates gas flows very accurately

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

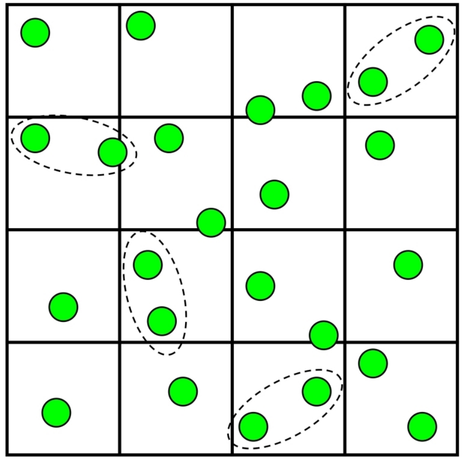
Computational and algorithmic advances have brought turbulent flows within reach of DSMC!

move



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

collide



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

What can we learn from molecular-level simulations of turbulence?

[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, …

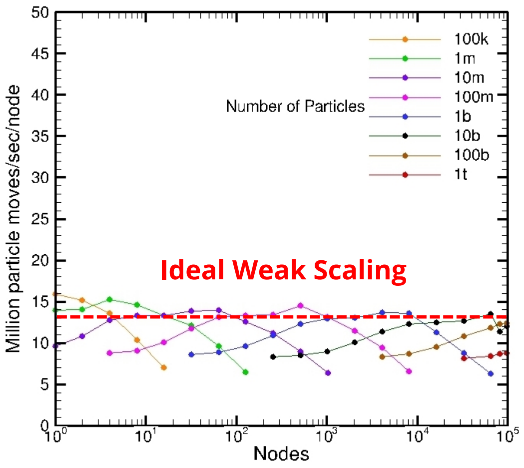
Complex geometries are easily treated

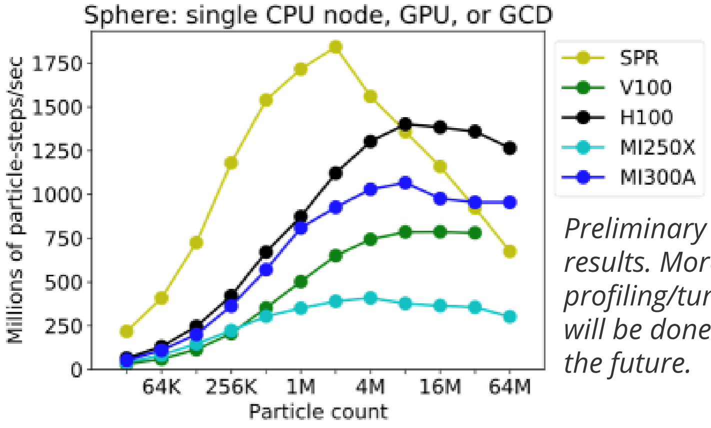
- Domain can be 2D, axisymmetric, 3D
- Gas molecules use hierarchical Cartesian grid
- Body surfaces represented by triangular elements which cut gas grid cells

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

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

More about SPARTA in Stan Moore's talk (session 17, 08:30)





Preliminary results. More profiling/tuning will be done in the future.

Flow over thermal-protection-system materials

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

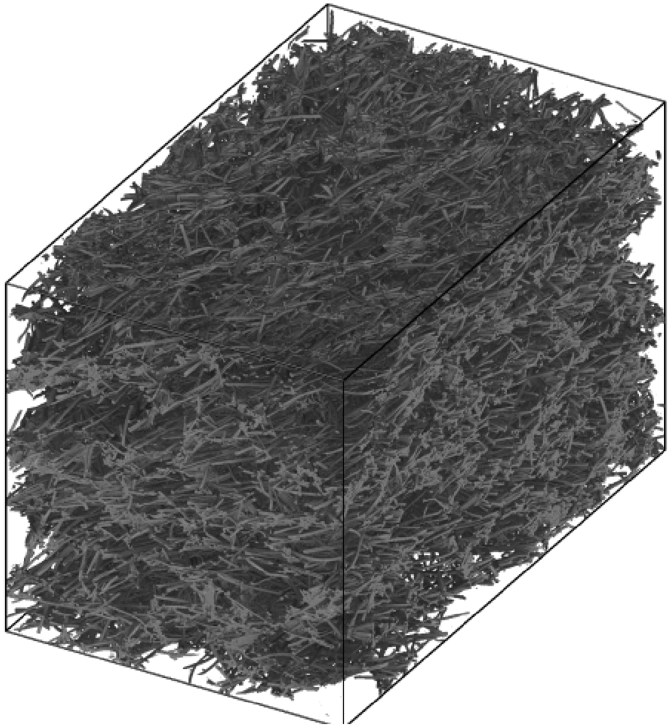
- Rough
- Permeable

→ Affects loading and may compromise vehicle performance

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

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

DSMC is well-suited for simulating flow over TPS materials!



3D scan of FiberForm™
(provided by NASA Ames)

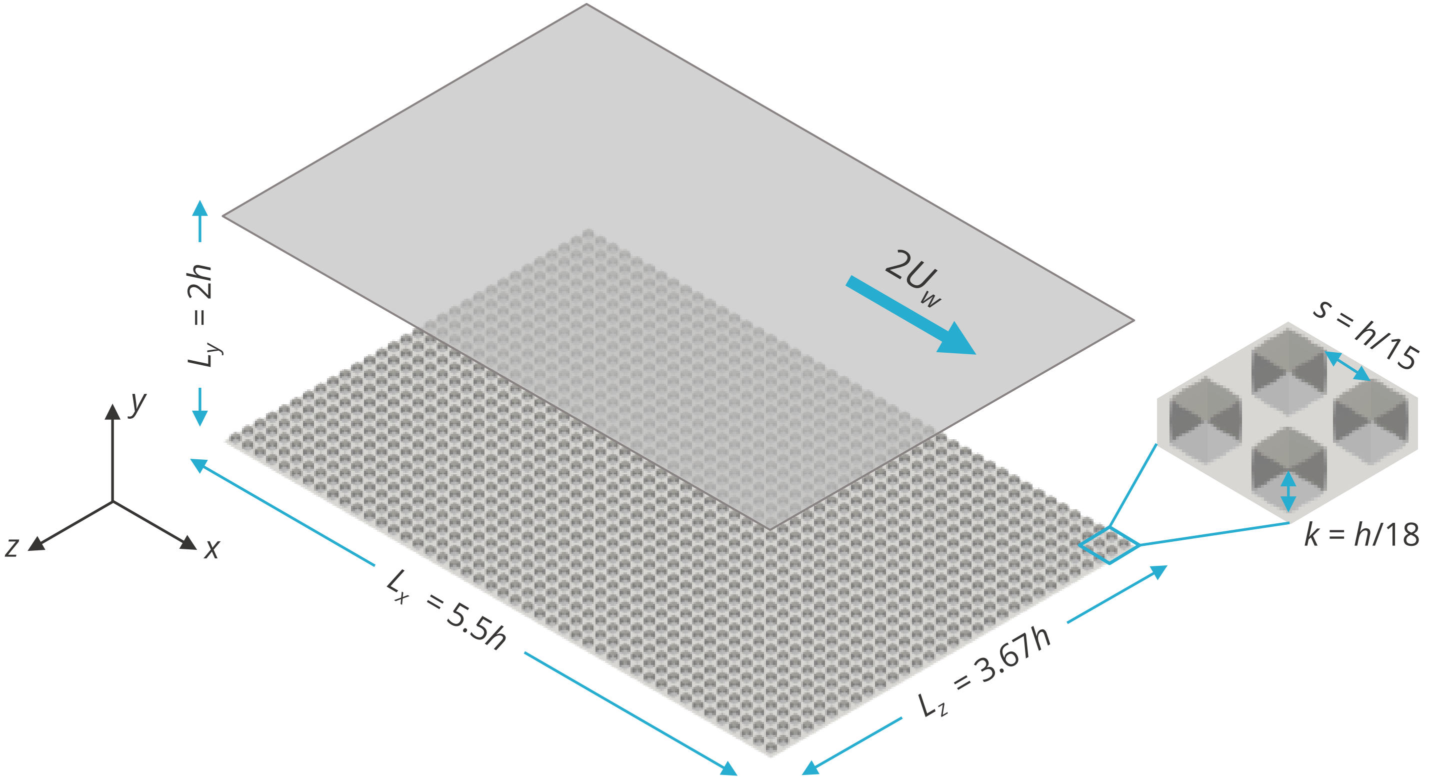
Goal: Simulate compressible turbulent flow over TPS-like rough and permeable walls with DSMC

First: Compare DSMC and CFD for rough-wall turbulence

Rough-wall turbulent Couette flow:

- Cuboidal roughness elements
- Small domain size
- Modest Reynolds number
- "Transitionally rough" regime
- Moderately compressible (no shocks)
- Near-continuum

DSMC and CFD should agree well for these conditions!



Ma	Re	Re_τ	k^+	Kn	$Kn_\tau = \lambda^+$
1.5	2800	210	11	8.7×10^{-4}	0.12

$Ma = U_w/a_w$

$Re = \rho_0 U_w h/\mu_w$

$Re_\tau = \rho_w u_\tau h/\mu_w$

$k^+ = \rho_w u_\tau k/\mu_w$

$Kn = \lambda_0/h$

$\lambda^+ = \rho_w u_\tau \lambda_w/\mu_w$

CFD simulations using SPARC

Direct numerical simulations (DNS) of the compressible Navier-Stokes equations

SPARC (Sandia Parallel Aerodynamics & Reentry Code)

- Compressible finite volume code

Blended flux scheme for high accuracy and stability

- 4th-order low-dissipation Subbareddy-Candler scheme in smooth regions
- 2nd-order dissipative modified Steger-Warming scheme near shocks
- Switch between schemes based on gradients in Mach number

4th-order Runge-Kutta time advancement

Simulation parameters for rough-wall turbulent Couette flow

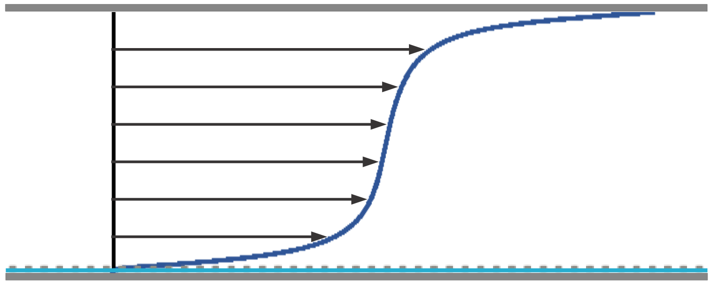
DSMC

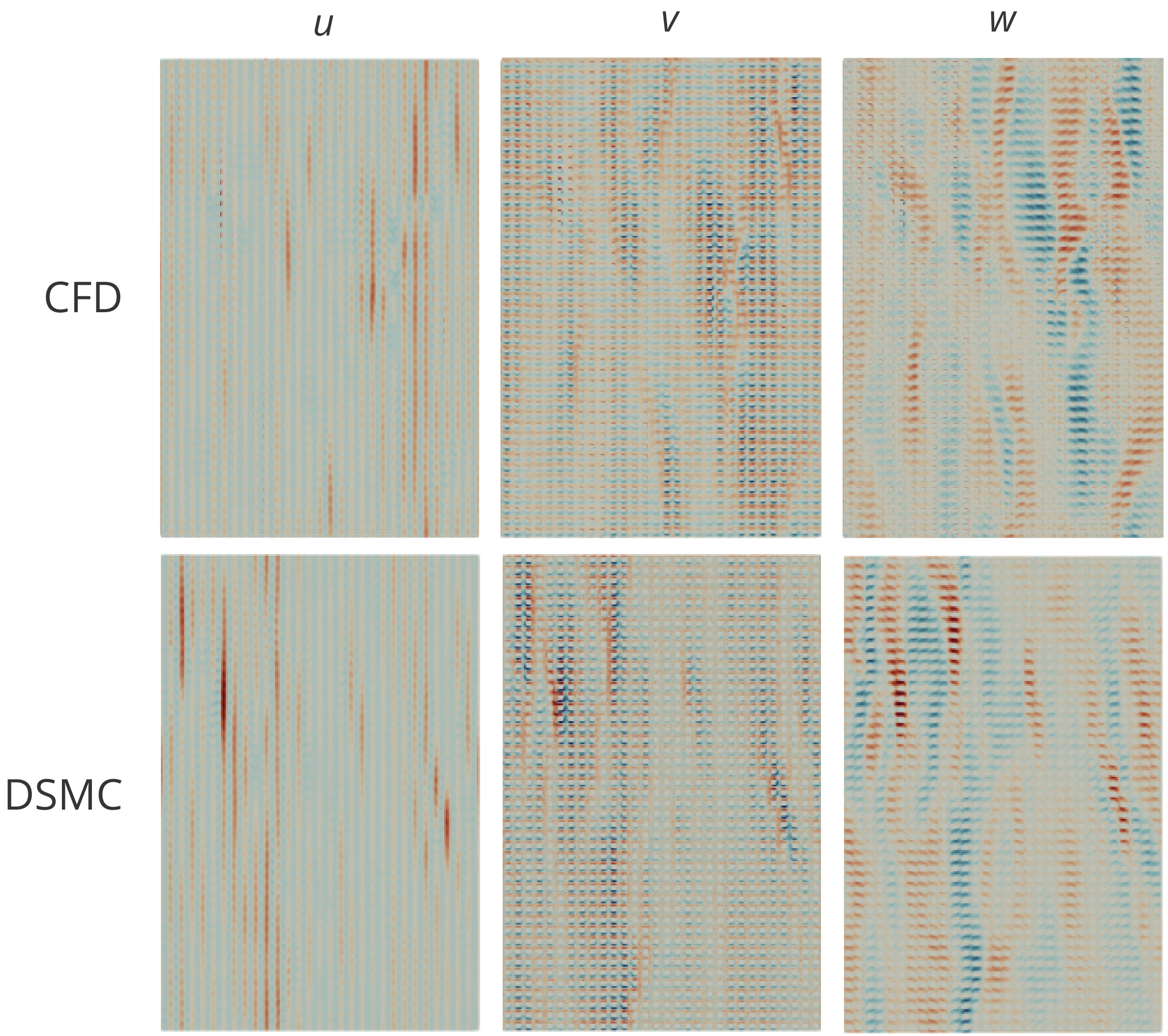
- Length scale: h = 500 μm
- Cell size: 1.3 μm
- Total cells: 2.6×10^{9}
- Total particles: 73×10^{9}
- Particles per cell: 28
- Time step: 9.1 ps
- Monatomic gas: $\gamma = 5/3$
- Molecular mass: 66.3×10^{-27} kg
- VSS collisions
- Near-neighbor algorithm
- BCs:
  - Walls: diffuse, $\alpha = 1$, T_w = 273.15 K
  - Periodic in x and z directions

CFD

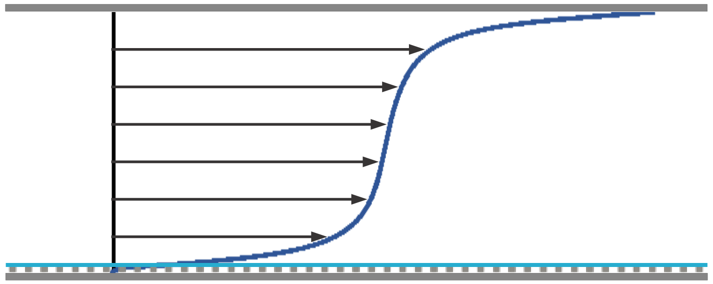
- Length scale: h = 1 m
- Cell sizes:
  - $\Delta x^+ = \Delta z^+ = 2$
  - Δy^+ = 0.4-4
- Time step: global CFL 0.25-0.5
- Ideal gas: $\gamma = 5/3$
- Power-law viscosity: $\mu/\mu_w = (T/T_w)^{0.5}$
  - μ_w set to value from DSMC calibration
- BCs:
  - Walls: no-slip, T_w = 273.15 K
  - Periodic in x and z directions

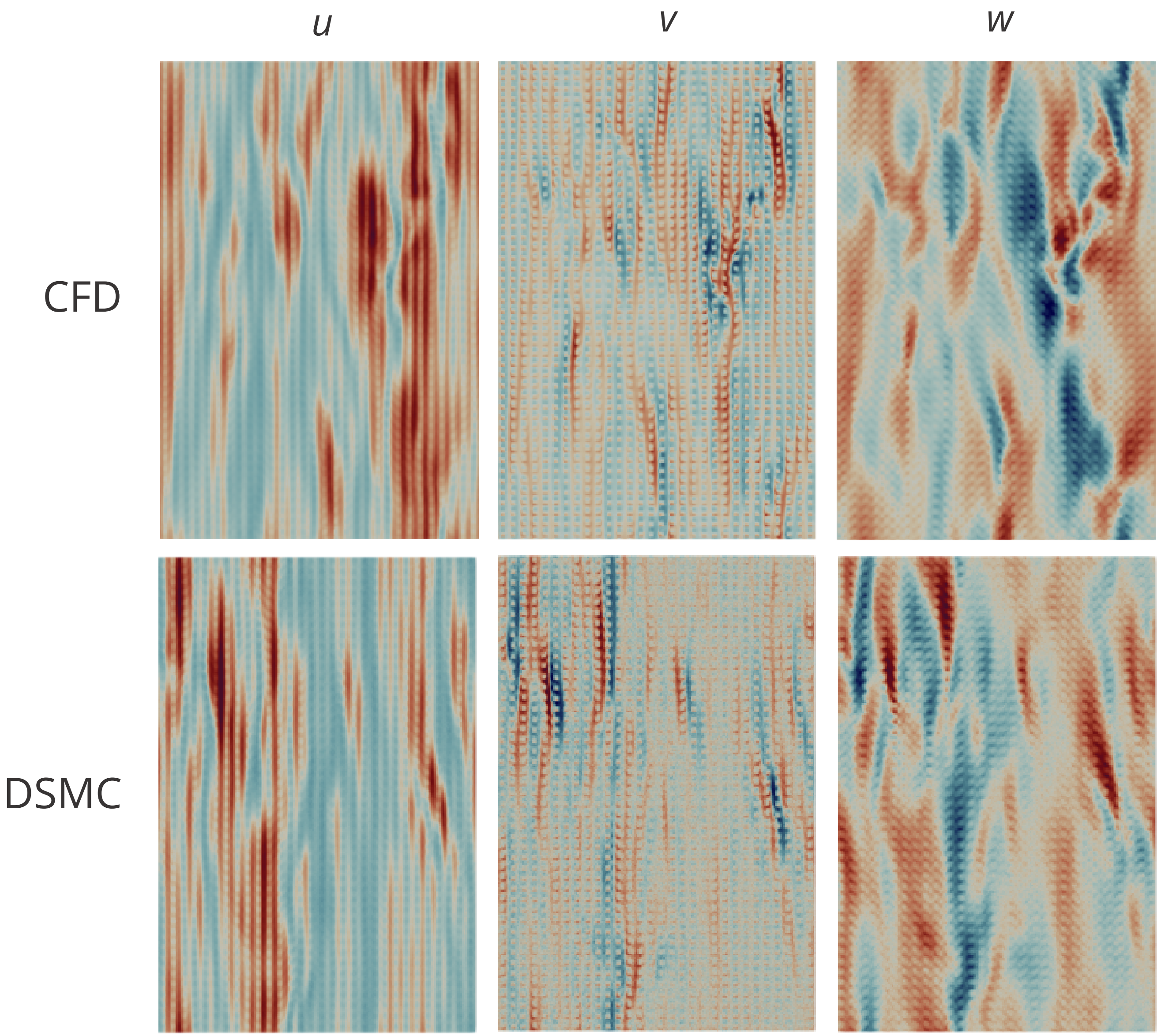
Flow structures: mid-cube



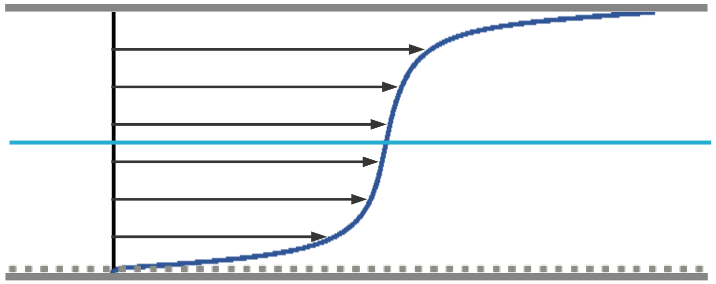


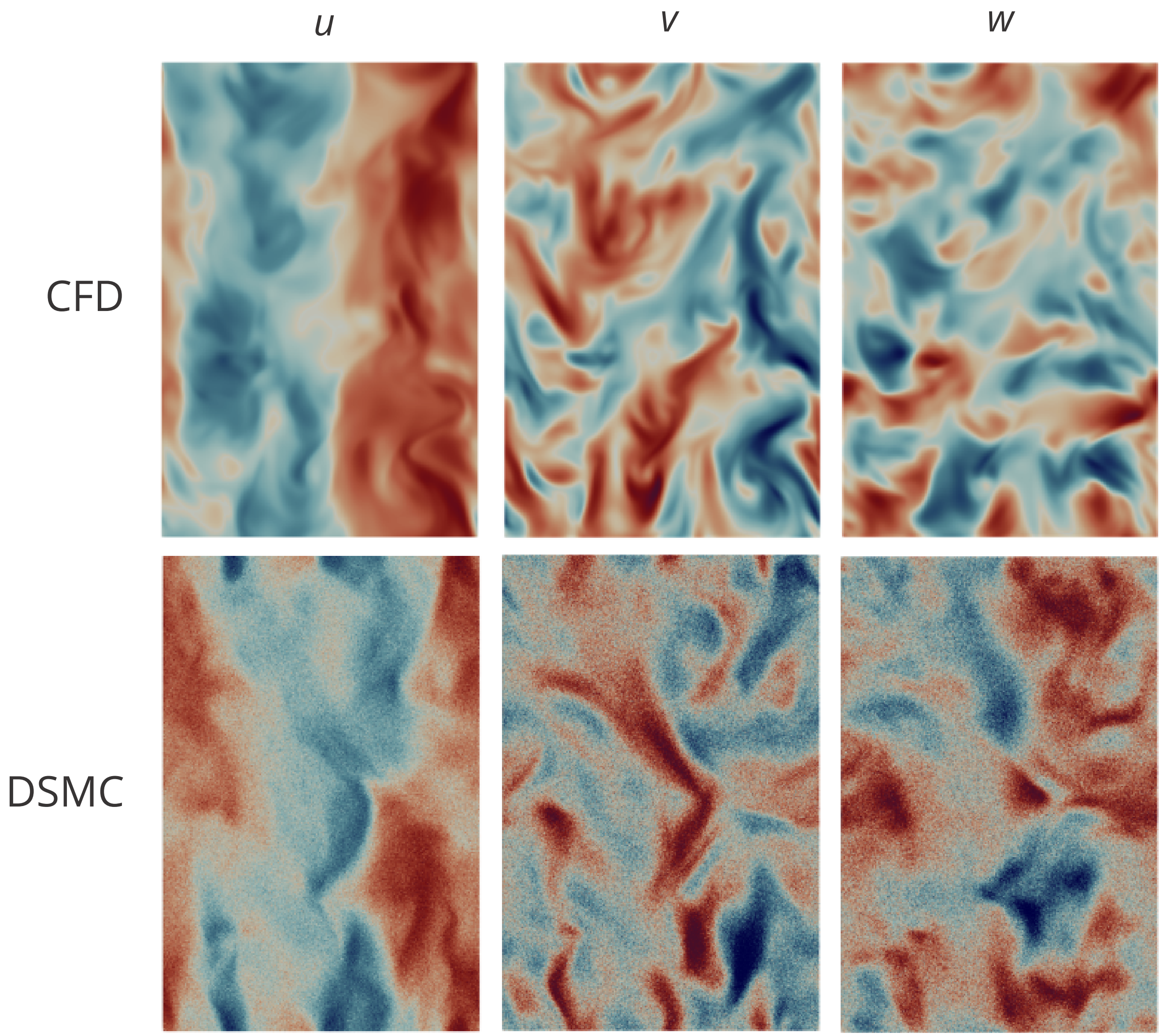
Flow structures: cube top



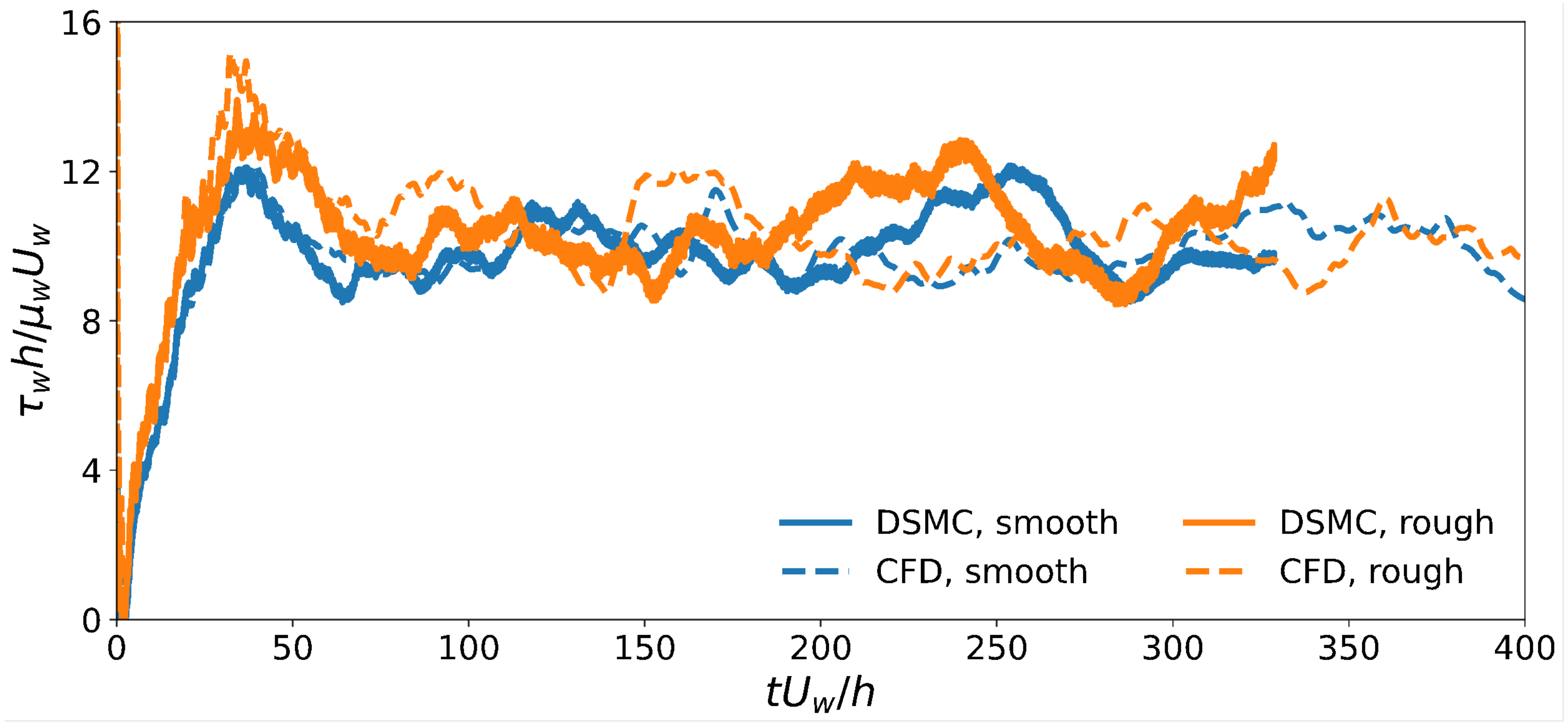


Flow structures: channel center





Skin friction

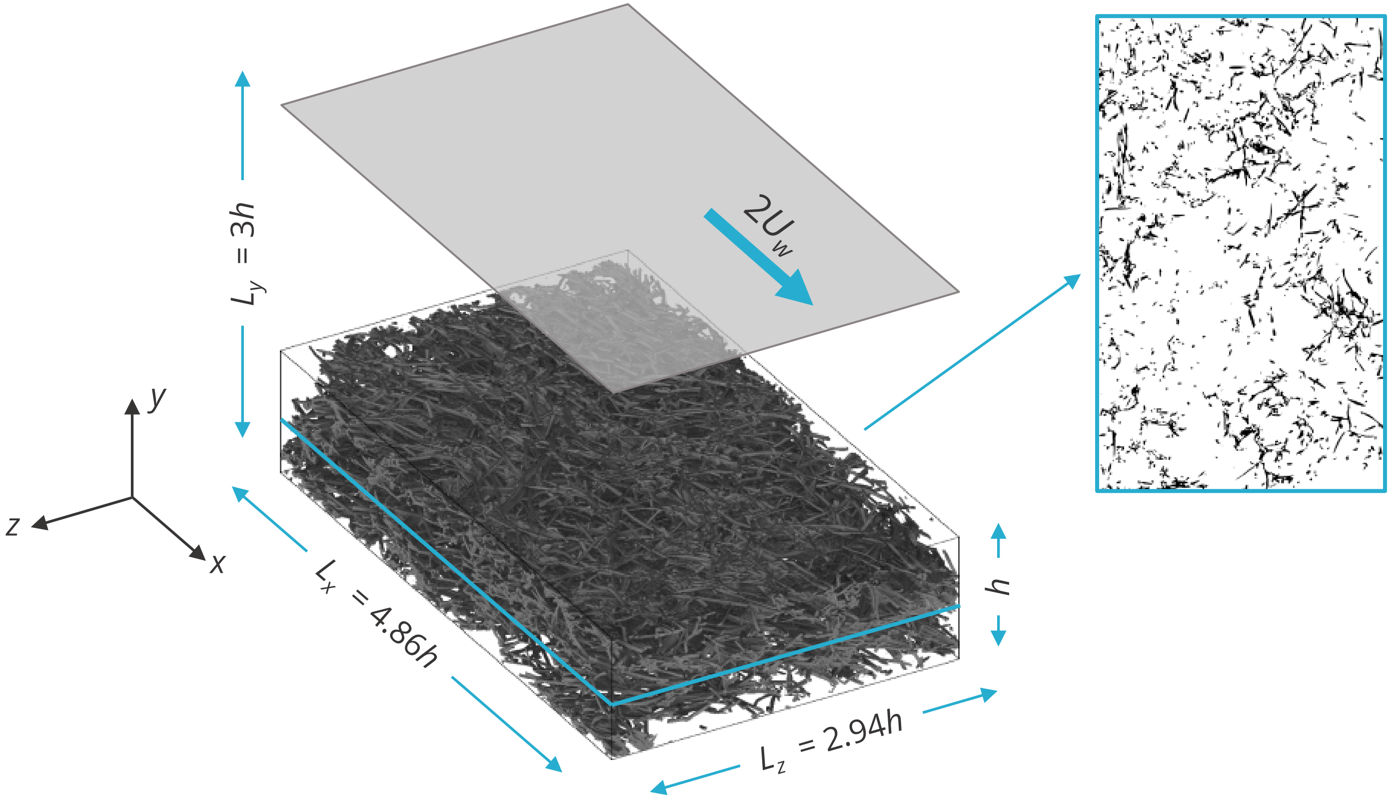


Time-averaged skin friction ($tU_w/h \geq 100$)

Surface	DSMC	DNS
Smooth	10.1	10.1
Rough	10.5	10.1

DSMC turbulent Couette flow over TPS material

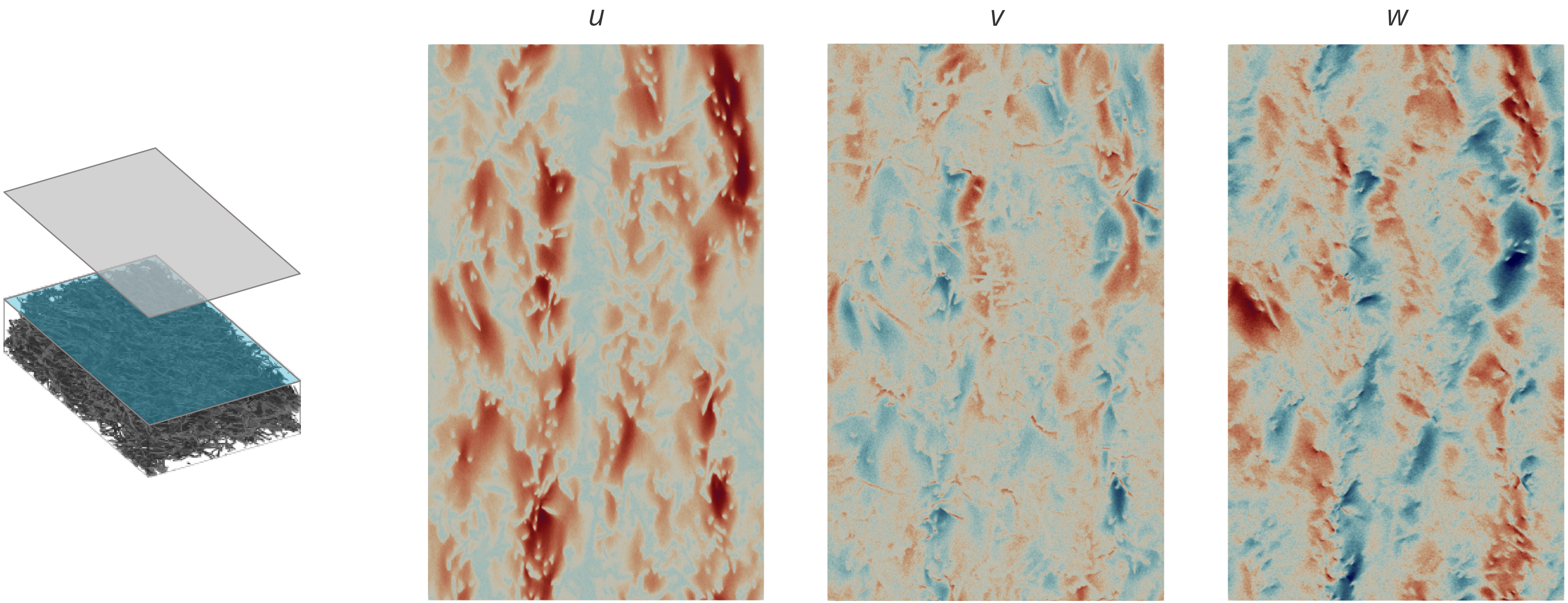
- Length scale: h = 500 µm
- Cell size: 1.7 µm
- Total cells: 1.2×10^9
- Total particles: 34×10^9
- Particles per cell: 29
- Time step: 9.1 ps
- Monatomic gas: $\gamma = 5/3$
- Molecular mass: 66.3×10^{-27} kg
- VSS collisions
- Near-neighbor algorithm
- BCs:
  - Walls: diffuse, $\alpha = 1$, $T_w = 273.15$ K
  - Periodic in x and z directions



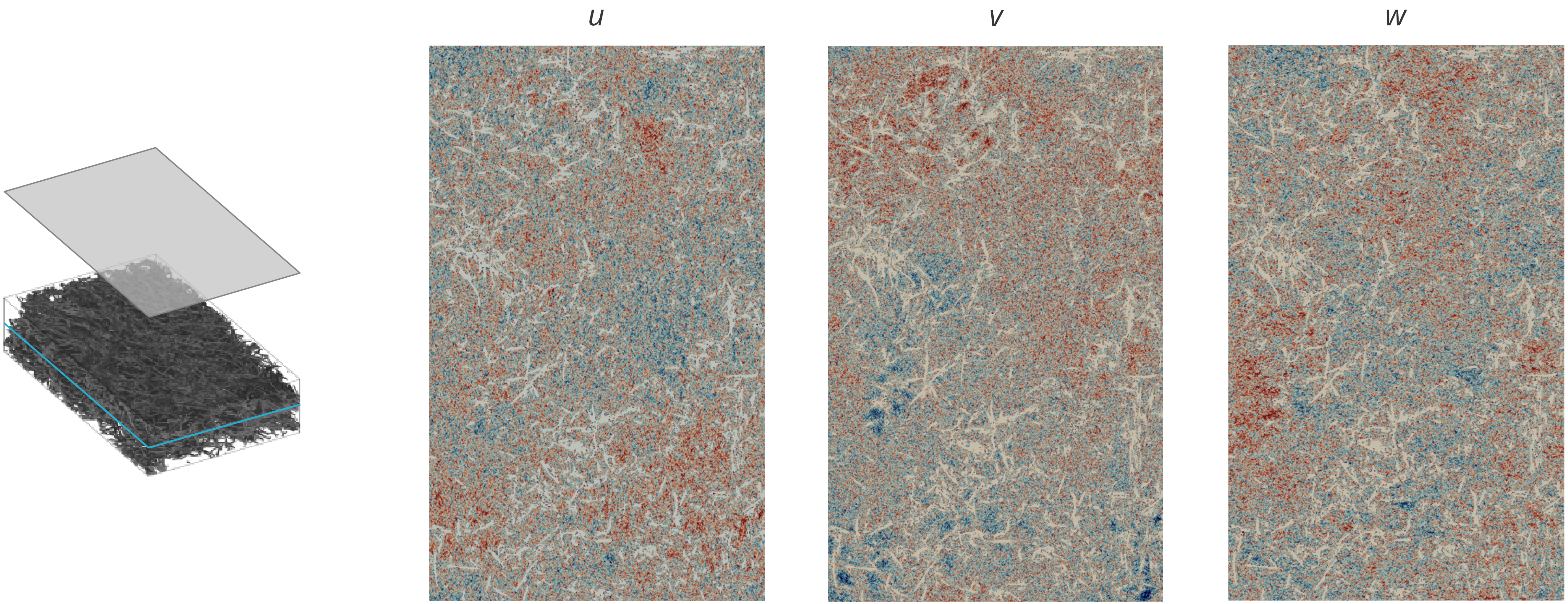
Ma	Re	Kn	ε	K_x/h^2	K_y/h^2	K_z/h^2
1.5	2800	8.7×10^{-4}	~0.9	$\sim4\times10^{-4}$	$\sim2\times10^{-4}$	$\sim4\times10^{-4}$

$\text{Ma} = U_w/a_w$ $\text{Re} = \rho_0 U_w h/\mu_w$ $\text{Kn} = \lambda_0/h$

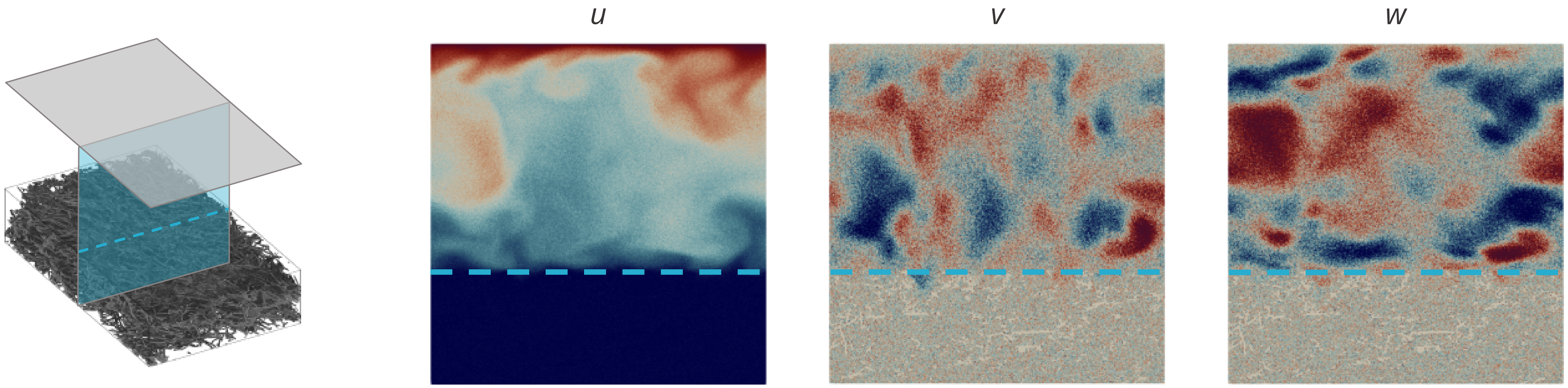
Flow structures: surface top



Flow structures: mid-surface



Flow structures: spanwise-wall-normal plane



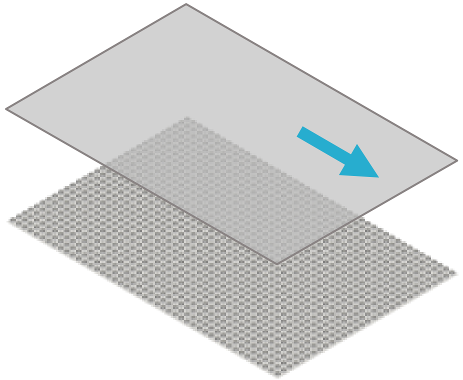
Summary

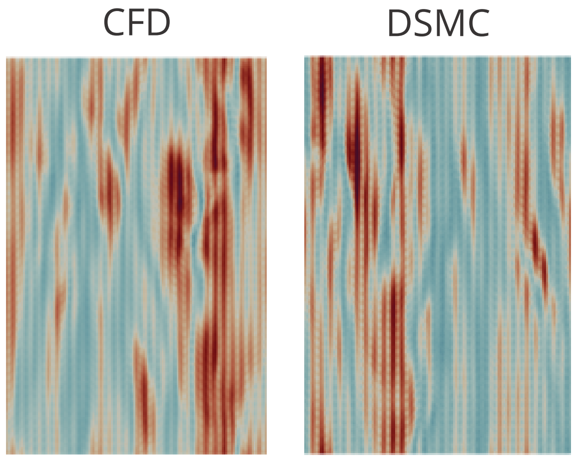
Preliminary comparison between DSMC and CFD for rough-wall turbulent Couette flow

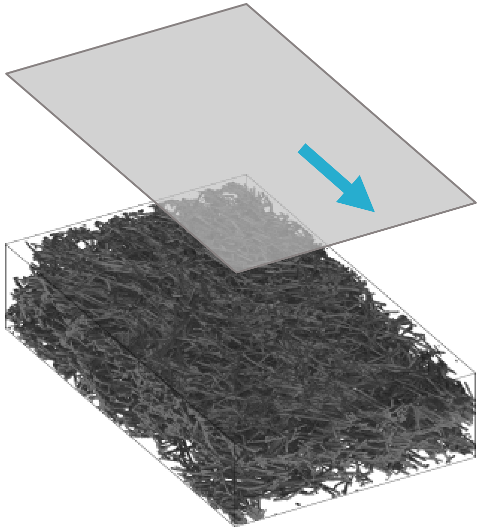
- Qualitatively similar flow structures
- Good quantitative agreement for skin friction
- Future work: quantitative comparison of turbulence statistics

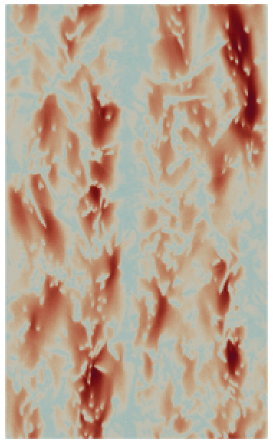
Preliminary DSMC investigation of turbulent flow over a 3D scan of real TPS material

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

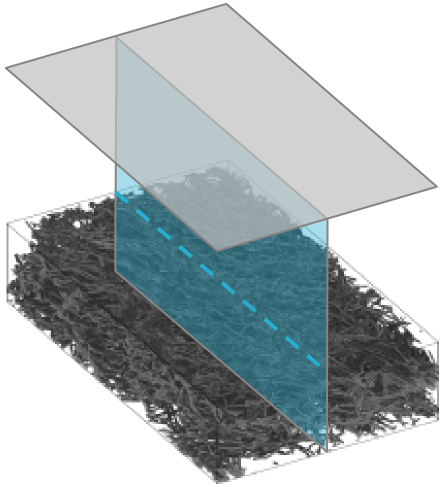


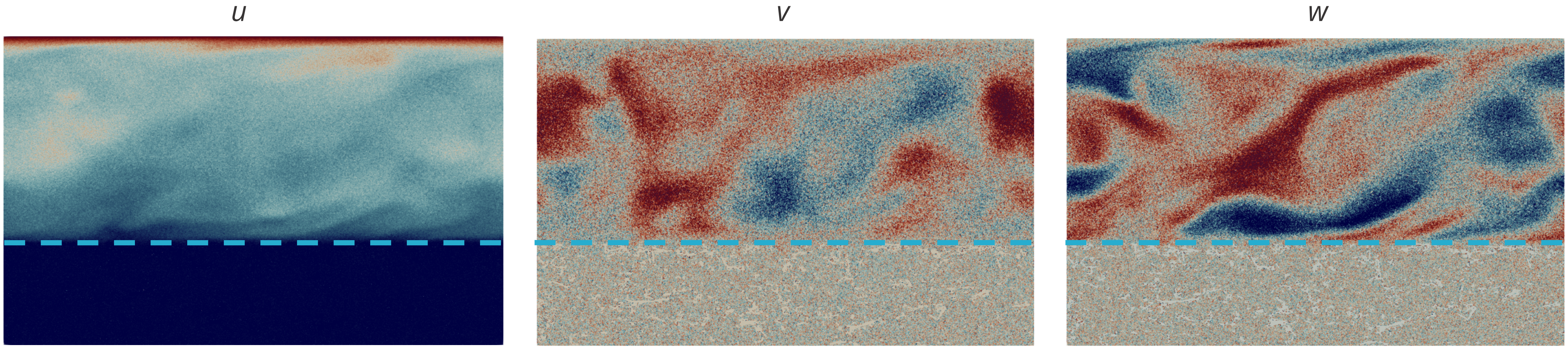






Flow structures: streamwise-wall-normal plane





Rough-wall time-averaged velocity profiles