Computational Flow Physics Laboratory
Apte Research Group

Turbulent Transport Across the Sediment-Water Interface: Pore-Resolved Direct Simulations and Upscaled Modeling

Sourabh V. Apte, Shashank Karra
Oregon State University

REMPLEX 2023 SUMMIT
PACIFIC NORTHWEST NATIONAL LABORATORY
NOV 13-17

Funding: DoE BES, PNNL (student internship), NSF

Background

- Hyporheic exchange - a **bidirectional** exchange of water, oxygen, pollutants, nutrients and energy between stream flow and sediments
- Penetration of mean and turbulent flow within the porous bed and near bed pressure fluctuations primarily influence hyporheic exchange (Hester et al' 2017)
- Permeability Reynolds number (representing the ratio between permeability scale to viscous scale)

$$Re_K = {u_\tau \sqrt{K}}/{\nu}$$

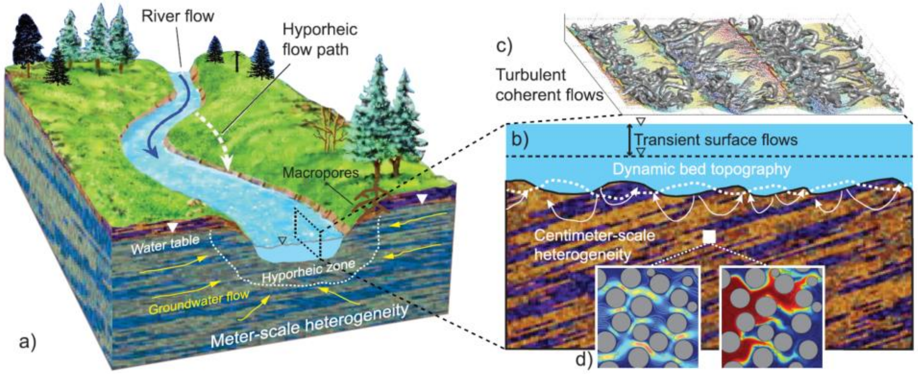
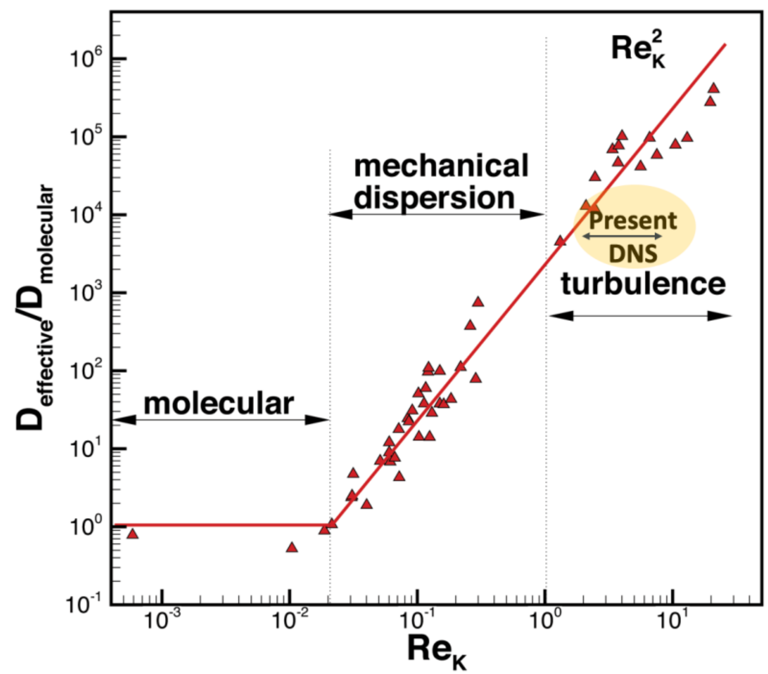


Figure taken from Hester et al' 2017



modified based on Voermans et al (JFM, 2017)

Objectives

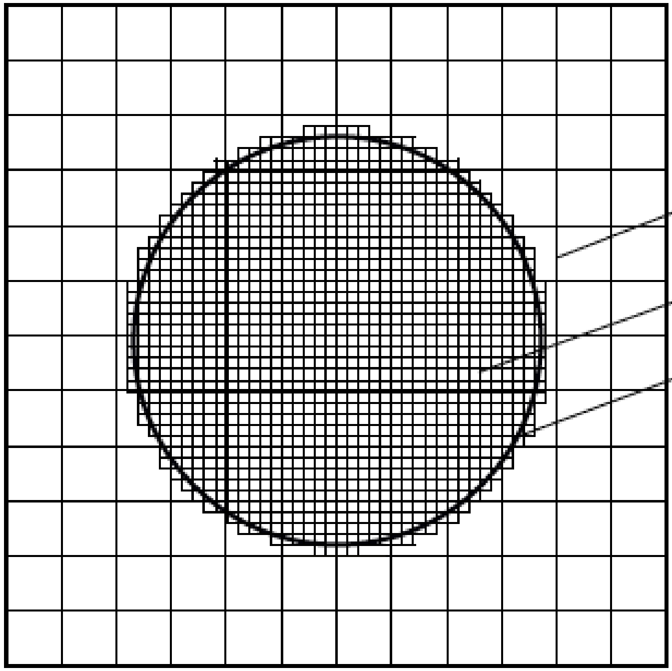
- Investigate the interactions between stream turbulence and groundwater flow through a randomly packed, porous sediment bed over a range of $Re_k \sim 2\text{-}10$ representative of stream flows
- Pore-resolved DNS to investigate turbulence characteristics in open channel flow over permeable beds
  - Fictitious domain method (Apte et al. 2008, Apte & Finn, 2012)
- Develop a diffuse interface based volume-averaged Navier-Stokes (VaNS) model and investigate its predictive capability compared to the pore-resolved DNS data
  - Volume-Averaged Navier-Stokes (VANS) Model (Whitaker 1996)
  - Closure for extra terms from volume averaging

Pore-Resolved Simulations: Fictitious Domain Method

$$\nabla \cdot \mathbf{u}_\gamma = 0$$

$$\rho_\gamma \left(\frac{\partial \mathbf{u}_\gamma}{\partial t} + (\mathbf{u}_\gamma \cdot \nabla)\, \mathbf{u}_\gamma \right) = -\nabla p + \mu_\gamma \nabla^2 \mathbf{u}_\gamma + \rho_\gamma \mathbf{g} + \mathbf{f}$$

Rigidity constraint force
Non-zero within the solid



- Navier-Stokes equations are solved over the entire domain (including the solid region)
- Rigidity constraint force **f** is used to impose rigid body motion within the solid region (no-slip on the boundaries and no deformation within the solid)
- Fractional time-stepping, collocated grid algorithm for overall second-order accuracy

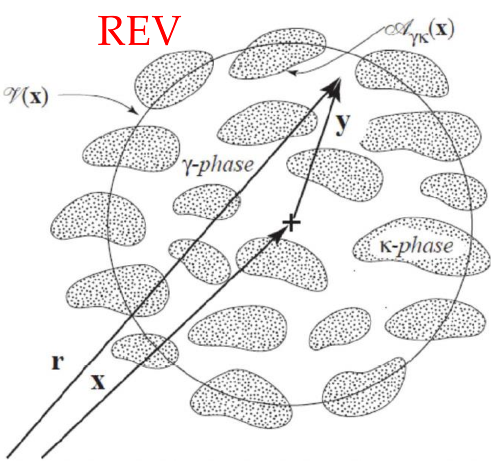
Apte et al. 2009 (JCP)
Apte and Finn 2013 (JCP)

Volume-averaged Navier Stokes (VANS)

- Volume averaging of any quantity ψ over a representative elementary volume (REV) can be written as

$$\langle \psi_\gamma \rangle = \frac{1}{V} \int_{\mathbf{r} \in \mathscr{V}(\mathbf{X})} I_\gamma(\mathbf{r}) \psi(\mathbf{r}) dV(\mathbf{r})$$

,



- Intrinsic volume average

$$\langle \psi_\gamma \rangle^\gamma = \frac{1}{V_\gamma} \int_{\mathbf{r} \in \mathscr{V}(\mathbf{X})} I_\gamma(\mathbf{r}) \psi(\mathbf{r}) dV(\mathbf{r})$$

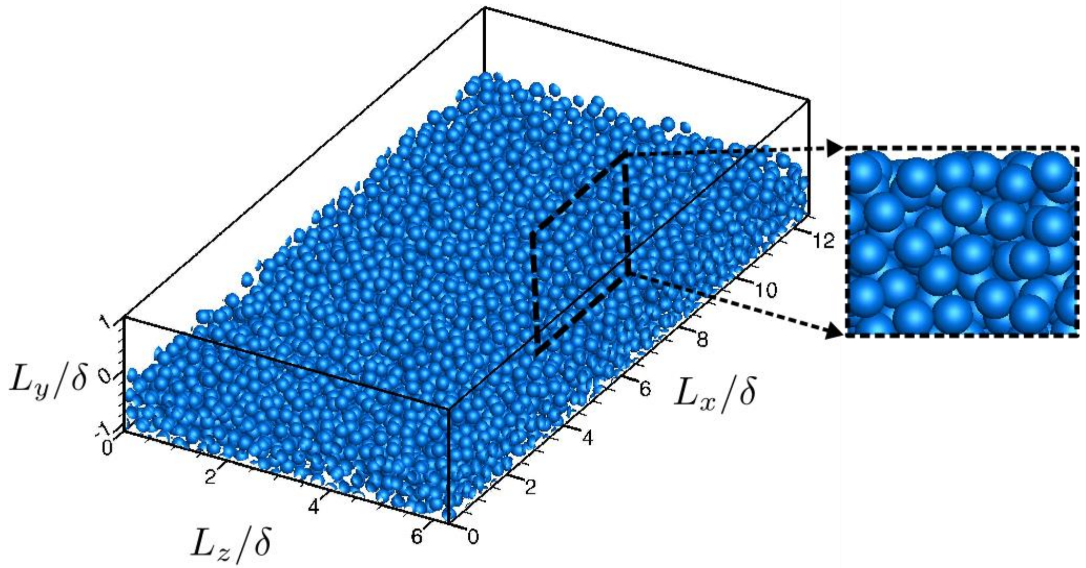
Whitaker, 1996
Wood, He, Apte 2020

porosity

$$\langle \psi_\gamma \rangle = \varepsilon_\gamma \langle \psi_\gamma \rangle^\gamma$$

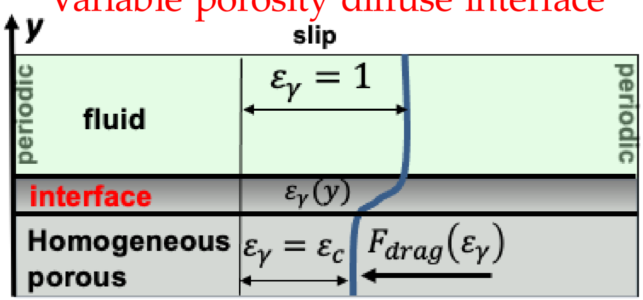
VaNS For Variable Porosity

PR-DNS

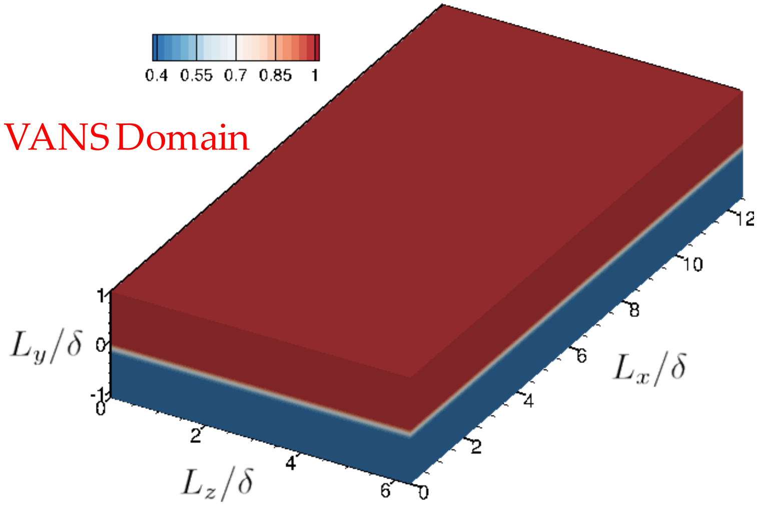


VANS model

Variable porosity diffuse interface



VANS Domain



Volume-averaged Navier Stokes (VANS)

Whitaker, 1996
Wood, He, Apte 2020

Spatially variable porosity

$$\nabla \cdot (\varepsilon_\gamma \langle \boldsymbol{u}_\gamma \rangle^\gamma) = 0$$

Intrinsic velocity field is not divergence free

Gradient diffusion hypothesis with eddy viscosity

$$\rho_\gamma \frac{\partial \varepsilon_\gamma \langle \boldsymbol{u}_\gamma \rangle^\gamma}{\partial t} + \rho_\gamma \nabla \cdot [\varepsilon_\gamma \langle \boldsymbol{u}_\gamma \rangle^\gamma \langle \boldsymbol{u}_\gamma \rangle^\gamma] + \underbrace{\rho_\gamma \nabla \cdot [\varepsilon_\gamma \langle \widetilde{\boldsymbol{u}}_\gamma \otimes \widetilde{\boldsymbol{u}}_\gamma \rangle]}_{\text{volume filter closure}} = -\nabla [\varepsilon_\gamma \langle p_\gamma \rangle^\gamma] +$$

$$\langle p \rangle_\gamma \nabla \varepsilon_\gamma + \mu_\gamma \nabla^2 [\varepsilon_\gamma \langle \boldsymbol{u}_\gamma \rangle^\gamma] - \mu_\gamma \nabla \varepsilon_\gamma \cdot \nabla \otimes \langle \boldsymbol{u}_\gamma \rangle^\gamma +$$

$$+ \underbrace{\frac{1}{V} \int_{A_{\gamma\kappa}} \mathbf{n}_{\gamma\kappa} \cdot (-\mathbf{I}\widetilde{p}_\gamma + \mu_\gamma \nabla \otimes \widetilde{\boldsymbol{u}}_\gamma) \mathbf{d}A}_{\text{surface filter closure}} + \rho_\gamma \varepsilon_\gamma \mathbf{f_b}$$

$$\frac{1}{V_\gamma} \int_{A_{\gamma\kappa}} \mathbf{n}_{\gamma\kappa} \cdot (-\mathbf{I}\widetilde{p}_\gamma + \mu_\gamma \nabla \otimes \widetilde{\boldsymbol{u}}_\gamma) \mathbf{d}A = -\mu_\gamma \mathbf{K}^{-1} (\mathbf{I} + \mathbf{F})$$

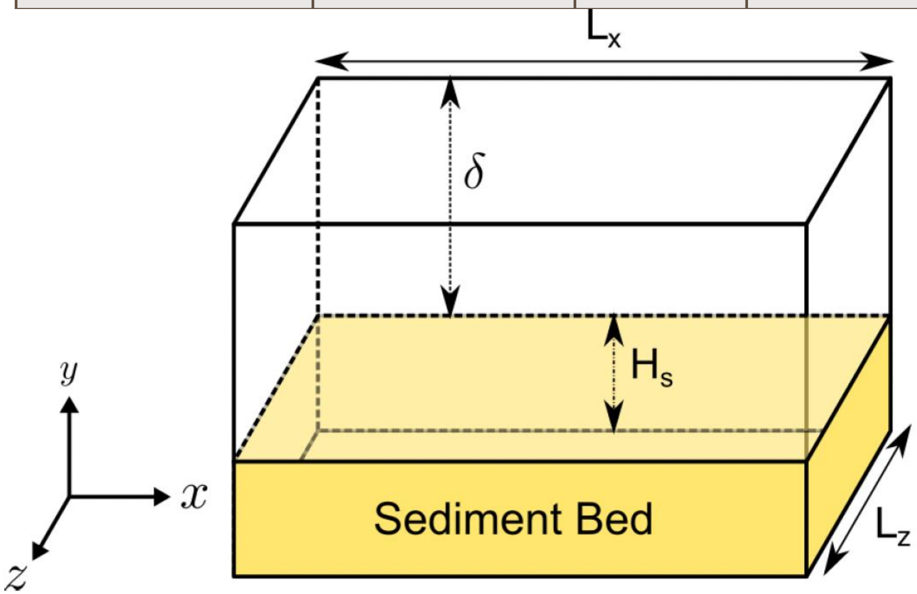
permeability (K) and Forchheimer (F) tensors

$$\mathbf{K} = \frac{d_p^2 \varepsilon_\gamma^3}{\mathcal{A}(1-\varepsilon_\gamma)^2} \mathbf{I}, \quad \mathbf{F} = \tilde{F} |\langle \boldsymbol{u}_\gamma \rangle^\gamma| \mathbf{I}, \quad \tilde{F} = \frac{\varepsilon_\gamma}{\mathcal{B}(1-\varepsilon_\gamma)} \frac{d_p}{\nu_\gamma}$$

Ergun model for packed beds

Cases studied and Parameters

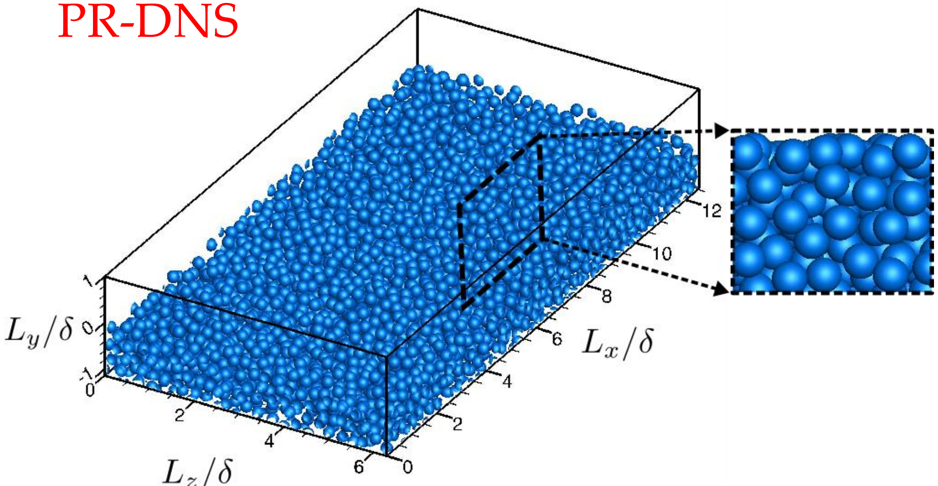
Case	Method	Re_K	Re_τ	θ	H_s/δ	D_p/δ	$(L_x, L_z)/\delta$
VV	PR-DNS	2.56	180	0.41	1.71	0.43	$(4\pi,2\pi)$
PBL	PR-DNS	2.56	270	0.41	1.14	0.29	$(4\pi,2\pi)$
PBM	PR-DNS	5.17	545	0.41	1.14	0.29	$(2\pi,\pi)$
PBH	PR-DNS	8.94	943	0.41	1.14	0.29	$(2\pi,\pi)$
PBL	VANS	2.5	263	0.41	1.14	-	$(4\pi,2\pi)$

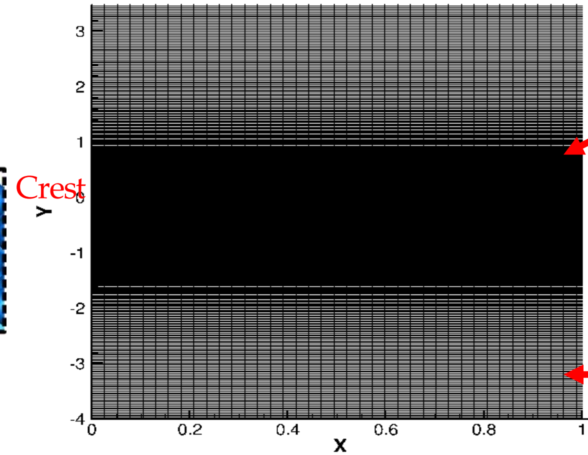


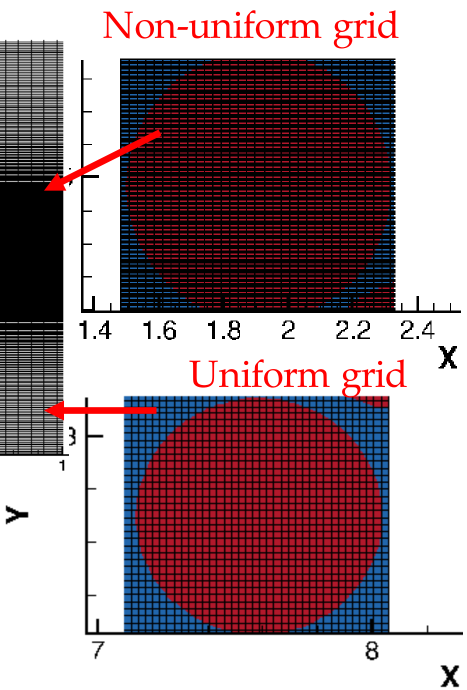
- **Cases**
  - **VV:** Verification and validation
  - **PBL,PBM,PBH:** Four layers of monodispersed spherical sediment particles for low, medium and high Reynolds number
  - VANS model: Diffuse interface based continuum approach

Sediment bed

PR-DNS







Random packing of mono-dispersed particles in doubly periodic domain generated using method of Dye et al. (2013)

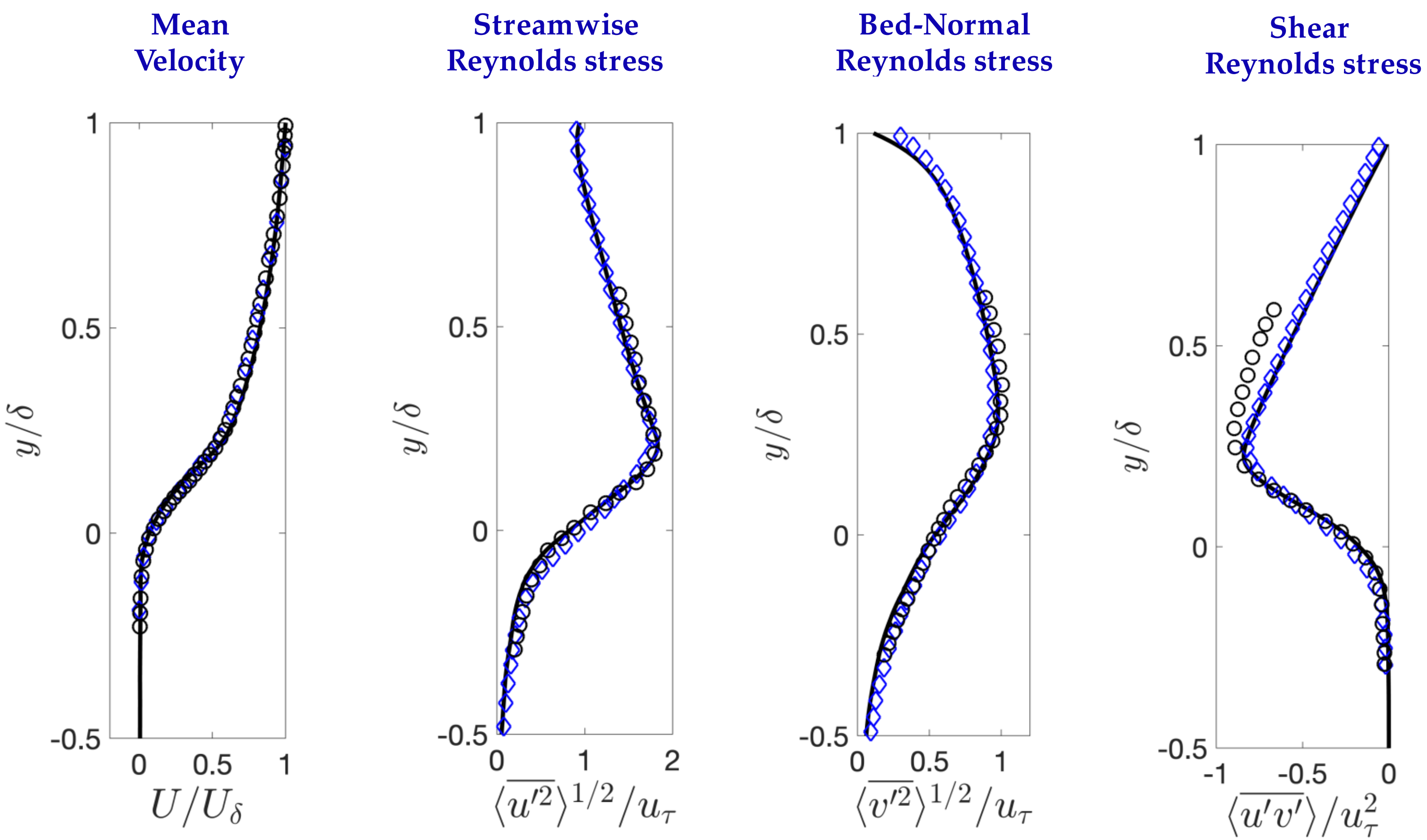
Grid distribution

Case	$N_x \times N_y \times N_z$	Bed-Normal Grid Distribution			$(\Delta x^+, \Delta y^+, \Delta z^+)$
		Channel region	Top layer	Bottom layers	
VV	$768 \times 288 \times 384$	96	86	106	(2.94, 0.95, 2.94)
PBL	$1152 \times 350 \times 576$	150	90	110	(2.94, 0.95, 2.94)
PBM	$846 \times 530 \times 448$	184	180	166	(4.01, 0.95, 3.8)
PBH	$882 \times 1082 \times 448$	342	548	192	(6.74, 0.55, 6.63)

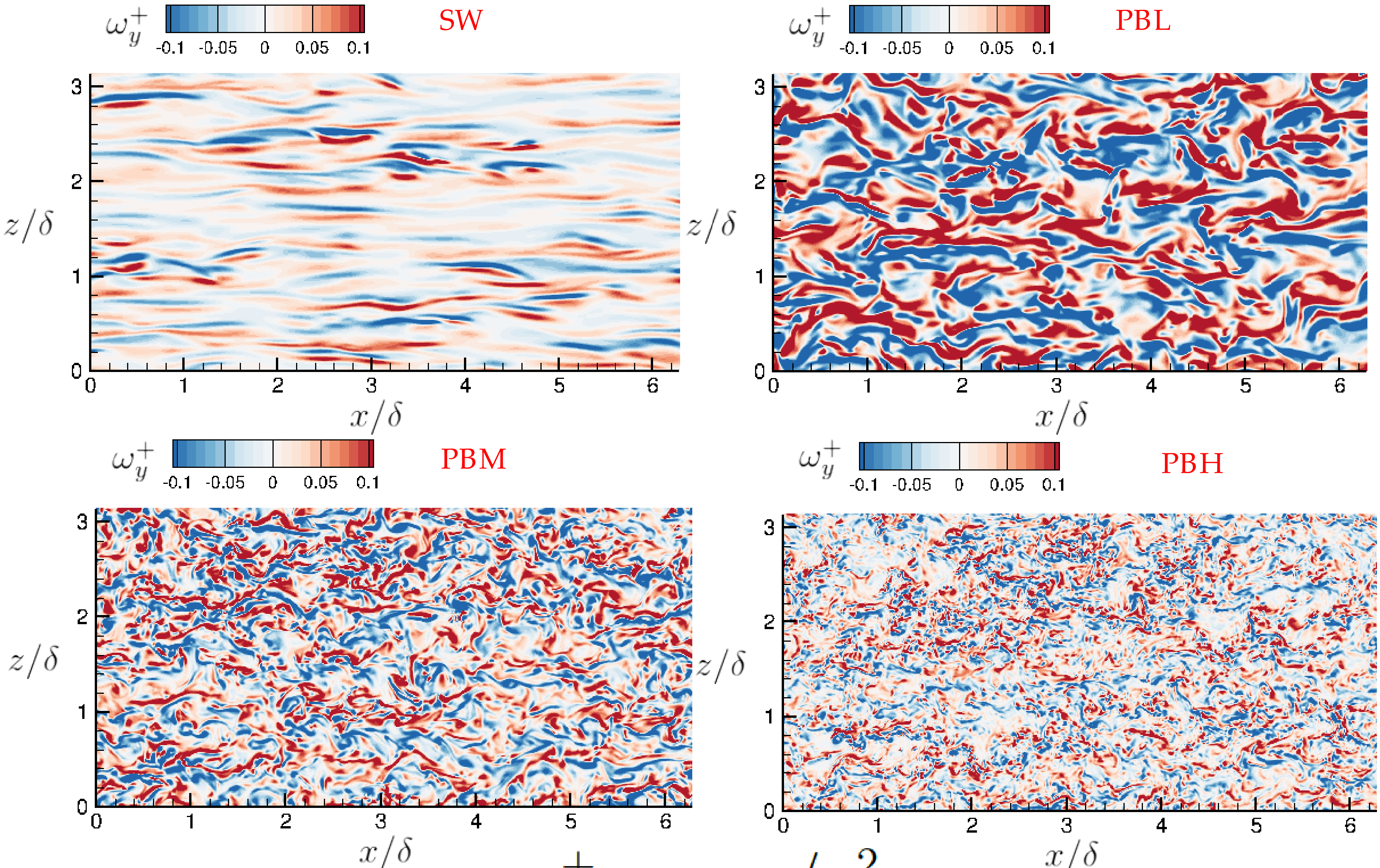
250M-500M cells. Computations done on Frontera on about 2000 processors

Pore-resolved DNS: Validation

- Pore-resolved DNS simulations (—) of turbulent flow over a sediment bed are validated with experimental data (o) from *Voermans et al., 2017 JFM* and DNS results (◇) from *Shen et al., 2019 JFM*
- Permeable bed $\theta = 0.41$, Re_K ~ 2.56, Re_τ = 180

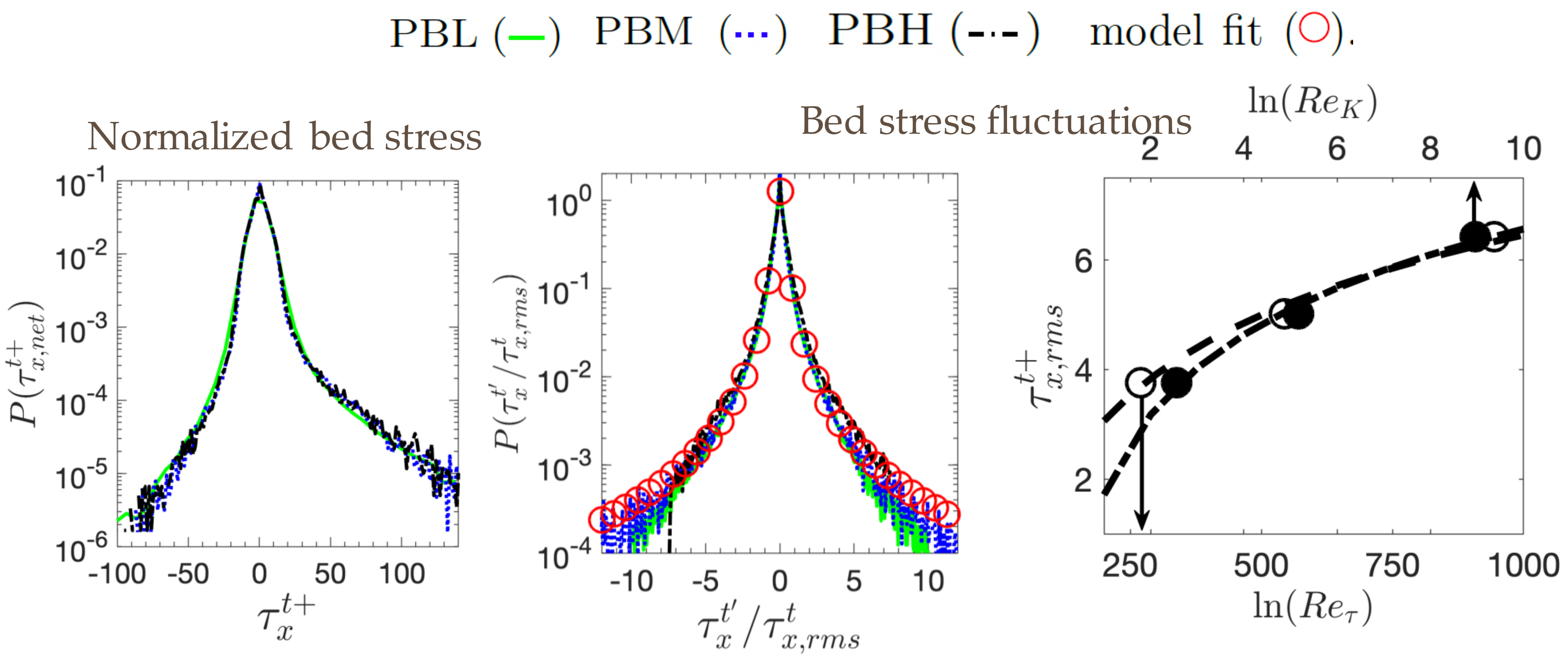


Turbulence structure (bed-normal vorticity)



$$\omega_y^+ = \omega_y \nu / u_\tau^2$$

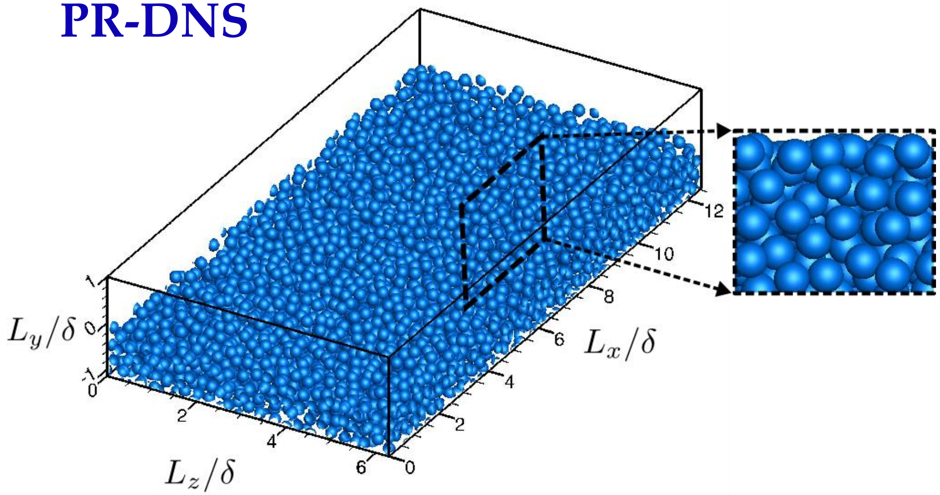
Net Bed Stress



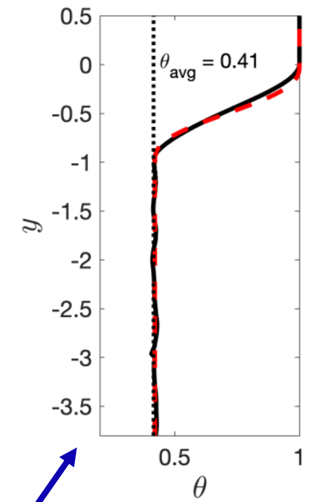
- PDFs of the local distribution of the net bed stress (pressure + viscous) normalized by the total bed stress in streamwise direction collapse for Re_K
- PDFs of the local distribution of fluctuations in net bed stress are symmetric, but non-Gaussian with heavy tails representative of extreme events
- Root mean square fluctuations of net bed stress follow a logarithmic correlation with Re_K

VaNS Model Setup

PR-DNS

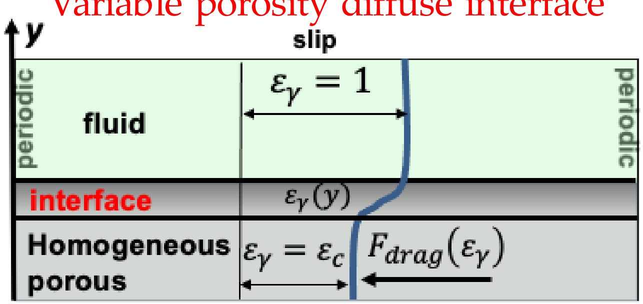


Porosity profile

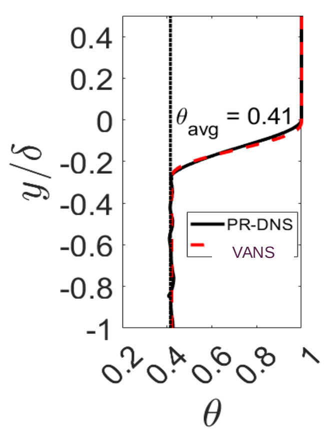


VANS model

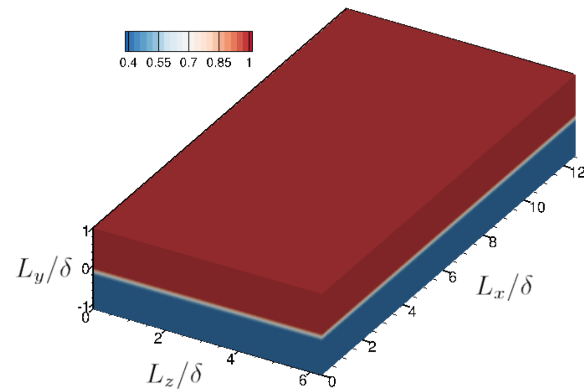
Variable porosity diffuse interface



Fifth-order polynomial fit



VANS Domain



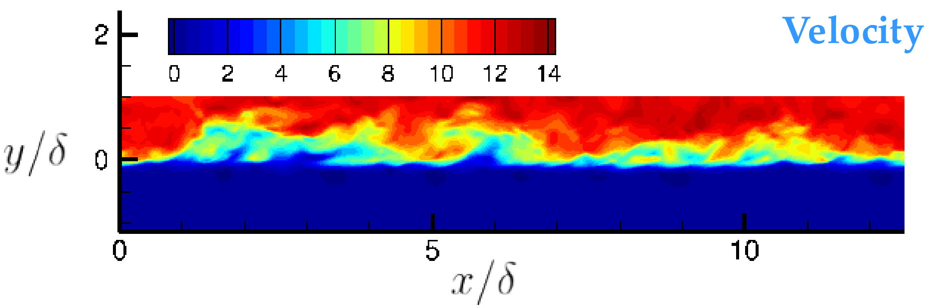
Turbulent flow comparison

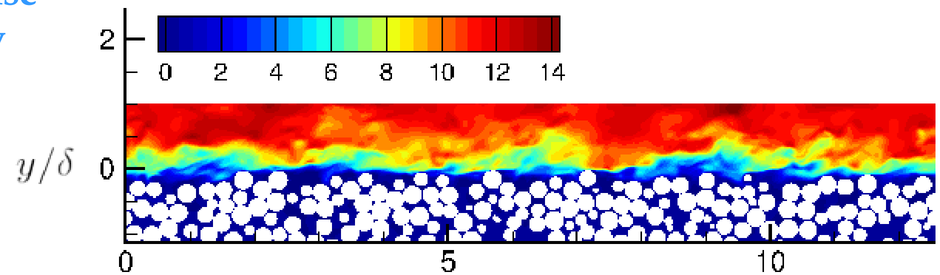
- Streamwise and bed-normal velocity at the z-symmetry plane
- A greater range of flow structures is observed in pore-resolved DNS

VANS-model

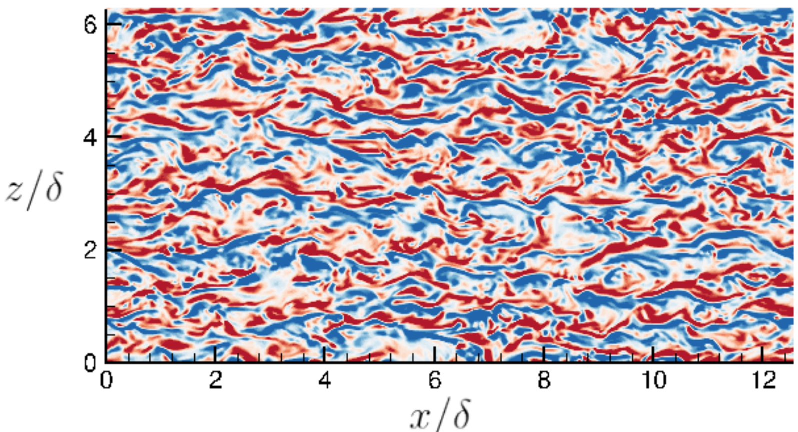
PR-DNS

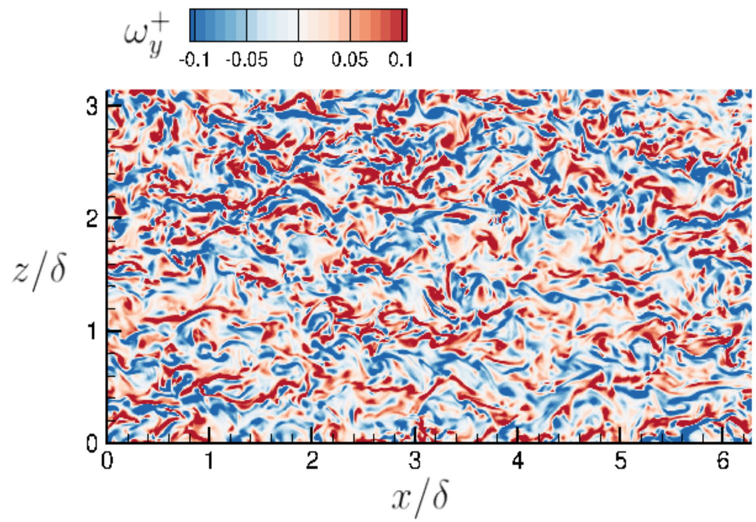
Streamwise Velocity





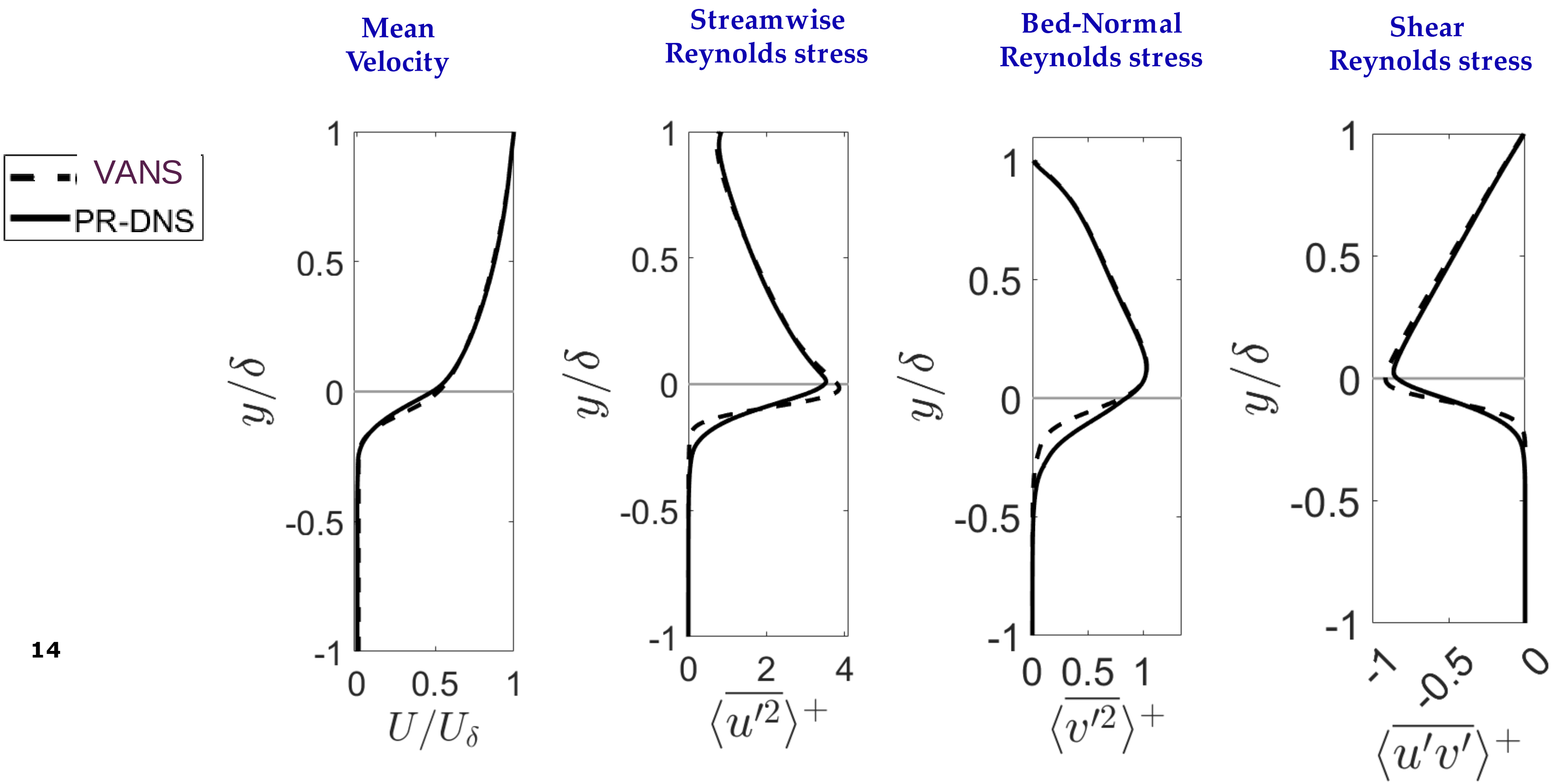
Bed-normal vorticity





Mean Velocity and Reynolds stresses

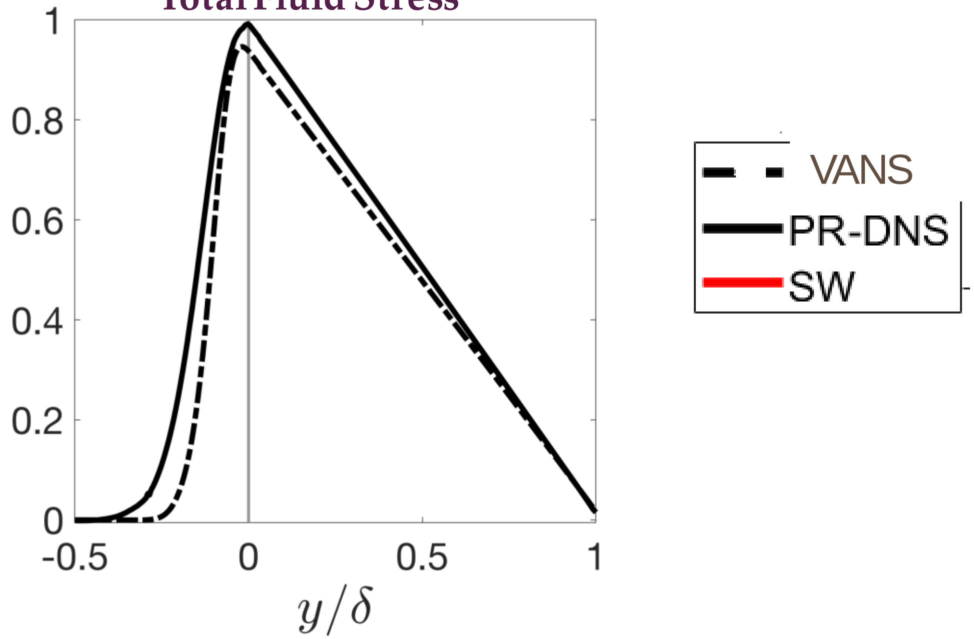
- Small differences near the crest and regions of rapid variations in porosity
- Attributed to effect of roughness protrusions on flow, which is absent in the continuum-based approach



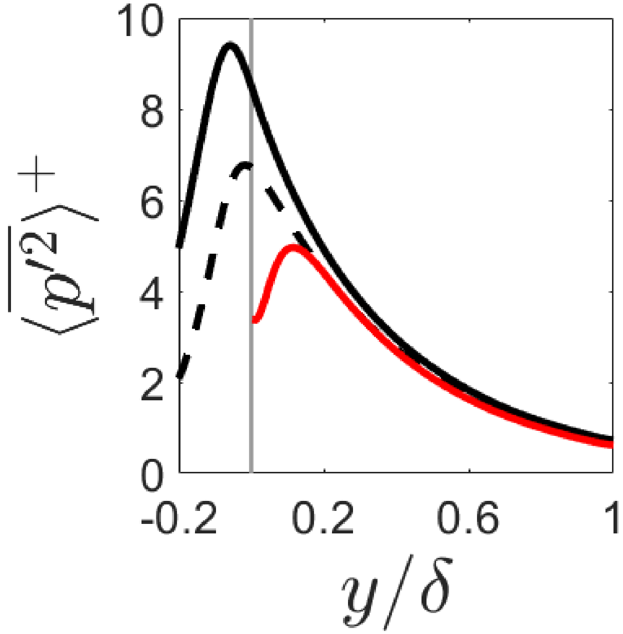
Total stress and pressure fluctuations

- Total fluid stress (viscous+turbulent+form-induced) is well captured
- Enhancement in pressure fluctuations in the top of the layer of the bed is observed in both cases compared to a smooth wall (red line)
- In pore-resolved DNS, the presence or roughness protrusions of the top layer clearly results in higher magnitude of pressure fluctuations. This behavior is not completely captured by continuum-based VaNS model
  - Future work: model variations in axial and spanwise porosity in the top layer

Total Fluid Stress



Pressure fluctuations



Conclusions

- Particle-resolved DNS and continuum VANS-based model were used to simulate free-stream turbulence over porous sediment bed and investigate turbulence penetration in the hyporheic zone
- Mean velocity, Reynolds stress, total fluid stress, and pressure fluctuations match well between the two approaches
- Enhancement in pressure fluctuations in the top of the layer of the bed is observed in both cases
- Lack of roughness protrusions in the VANS-model, result in underprediction of pressure fluctuations at the sediment-water interface
  - Better representation of the small-scale variations in porosity
  - Improved force closure in the varying porosity region
  - Scalar transport

- Thank you!