UQ+ML for turbulence models in CFD

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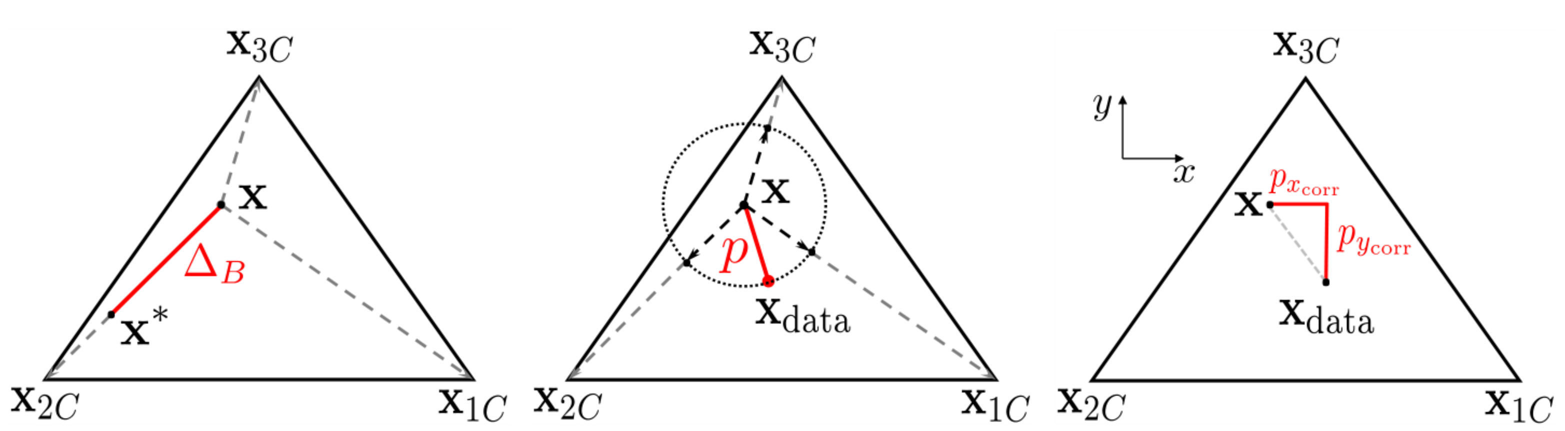
Need for UQ of turbulence models

Reynolds-averaged Navier-Stokes (RANS) simulation is the workhorse in industrial designs. The derivation of the RANS equations reveals an unclosed term, called the Reynolds stress tensor. This tensor has to be approximated in Computational-Fluid-Dynamics (CFD) simulations by applying turbulence models. Although RANS-based models, such as linear eddy viscosity models, are widely used for complex engineering flows, they suffer from the inability to replicate fundamental turbulent processes, reducing the prediction accuracy of the entire simulation. Assumptions, made during the formulation of turbulence models, lead to a significant degree of epistemic uncertainty. In this work, we investigated the possibility of uncertainty quantification (UQ) with DLR's CFD solver suite TRACE.

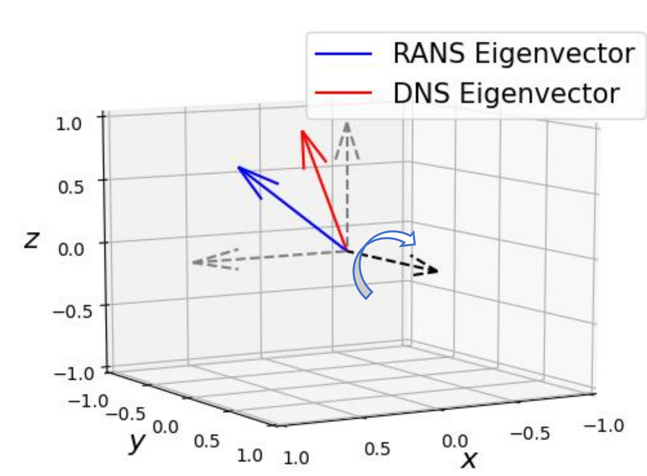
Reynolds stress eigenspace perturbation

Data-free & data-driven framework

RANS turbulence models are utilized in order to determine the Reynolds stress tensor $\tau_{ij} = k(a_{ij} + 2/3\delta_{ij}) = k(v_{in}\Lambda_{nl}v_{jl} + 2/3\delta_{ij})$, with k being the turbulent kinetic energy and the anisotropy tensor a_{ij}.
The eigenspace perturbation framework seeks to perturb the eigenvalues Λ and the eigenvectors v of the anisotropy tensor within physical limits [1].
The eigenvalues are modified by shifting their projection in terms of barycentric coordinates $\mathbf{x}$ towards the corners. The data-free approach uses a uniform relative distance Δ_B towards each corner and analyses the effect on the quantity of interest. A machine learning (ML) model should predict a local perturbation strength p in order to do the UQ analysis afterwards.
In a second step the model should also determine the actual correction $\mathbf{p}_{\mathrm{corr}}$ in terms of barycentric coordinates.
Additionally, the eigenvectors are modified by a rigid body rotation based on three intrinsic Tait-Bryan angles α, β, γ in order to fit the eigenvectors of high-fidelity data as well.



Schematic representation of the eigenvalue perturbation approach.
left: definition of perturbed state $\mathbf{x}^*$; middle: definition of perturbation strength p; right: definition of perturbation correction $\mathbf{p}_{\mathrm{corr}}$



Exemplary representation of the eigenvector misalignment. Rotation about y-Axis will map these vectors.

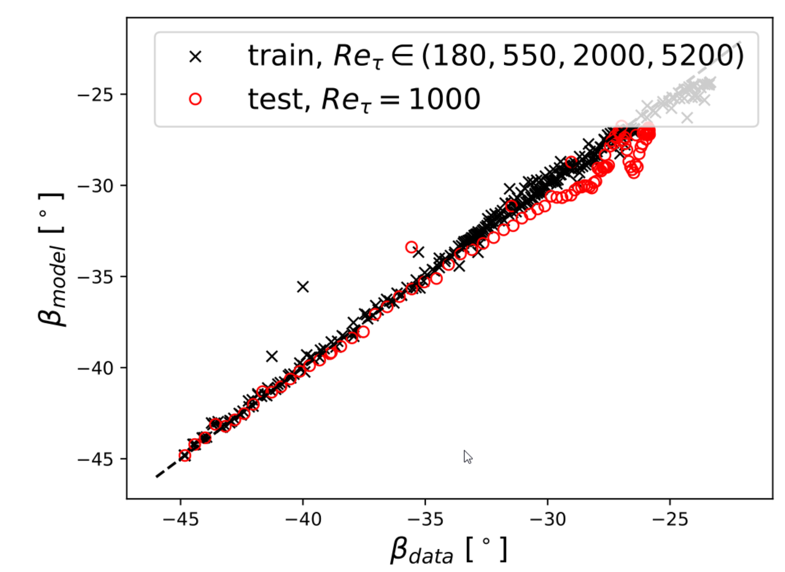
Random forest

Machine learning model

The python library *scikit-learn* is used to train the random forest and evaluate its prediction. In terms of selected flow features, we extended physically motivated quantities to the proposed exhaustive invariant feature list based other research [2][3].
The random forest regression models are trained on DNS data [4] of turbulent channel flow at $Re_\tau \in (180, 550, 2000, 5200)$ using the mean squared error to determine the quality of each split, whereas the models are evaluated in forward CFD-simulations at $Re_\tau = 1000$.

Selected hyperparameters for the random forest regressors

	Target quantities		
Hyperparameters	p	$\mathbf{p}_{\mathrm{corr}}$	$\mathbf{p}_{\mathrm{corr}} + \alpha, \beta, \gamma$
max tree depth	6	9	9
min sample count	6	4	4
max active features	3	3	3
number of trees	30	15	30

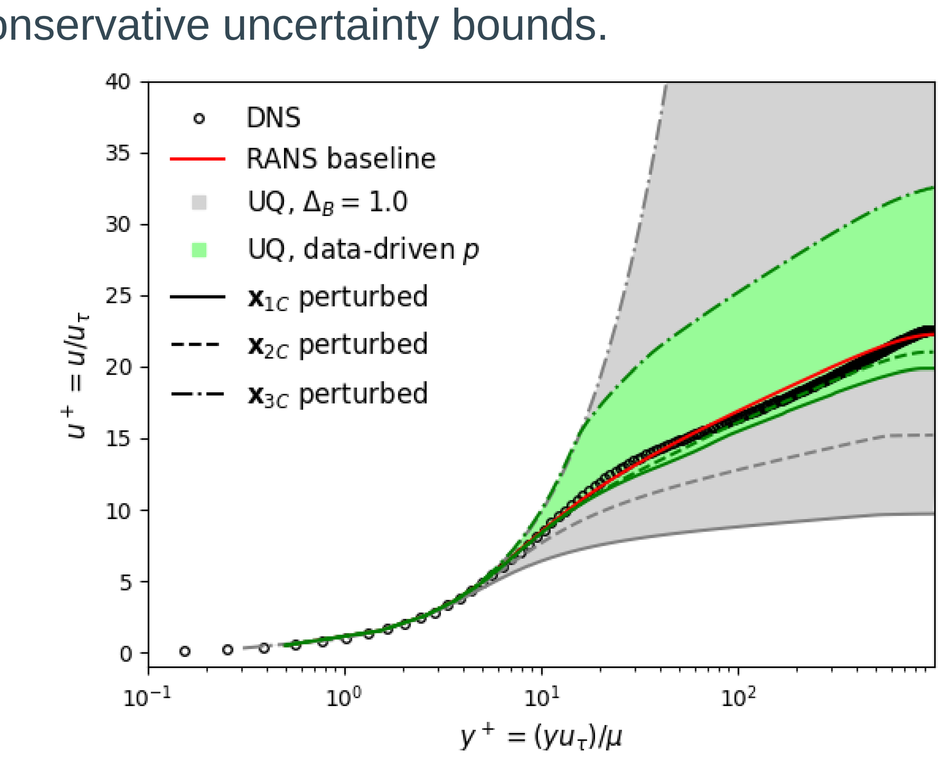


Exemplary analysis of the model accuracy for the prediction of an rotation angle

Advantage of data-driven eigenvalue UQ

Turbulent channel flow

The spatially varying perturbation strength p is predicted by the random forest and compared with a uniform perturbation based on the data-free method with chosen $\Delta_B = 1.0$. The data-driven perturbation approach reveals its superiority by determining more adequate perturbations, leading to less conservative uncertainty bounds.

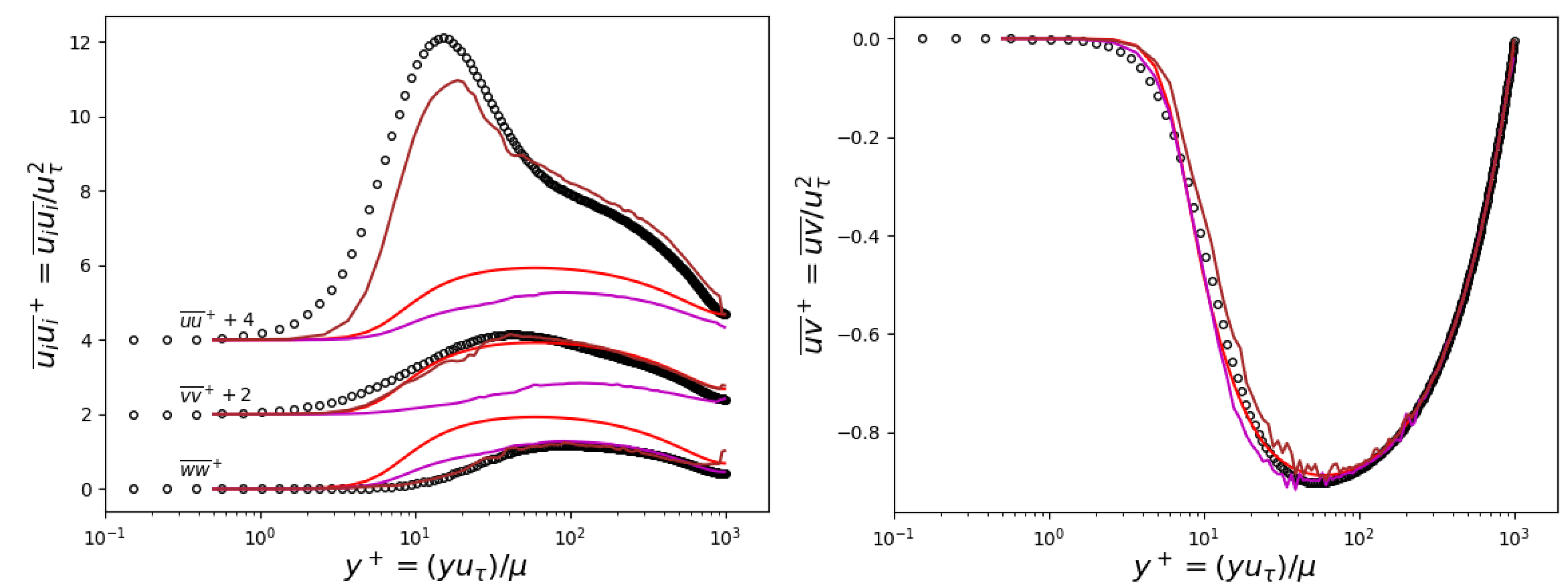


Determined uncertainty bounds for velocity profile of turbulent channel flow at $Re_\tau \approx 1000$

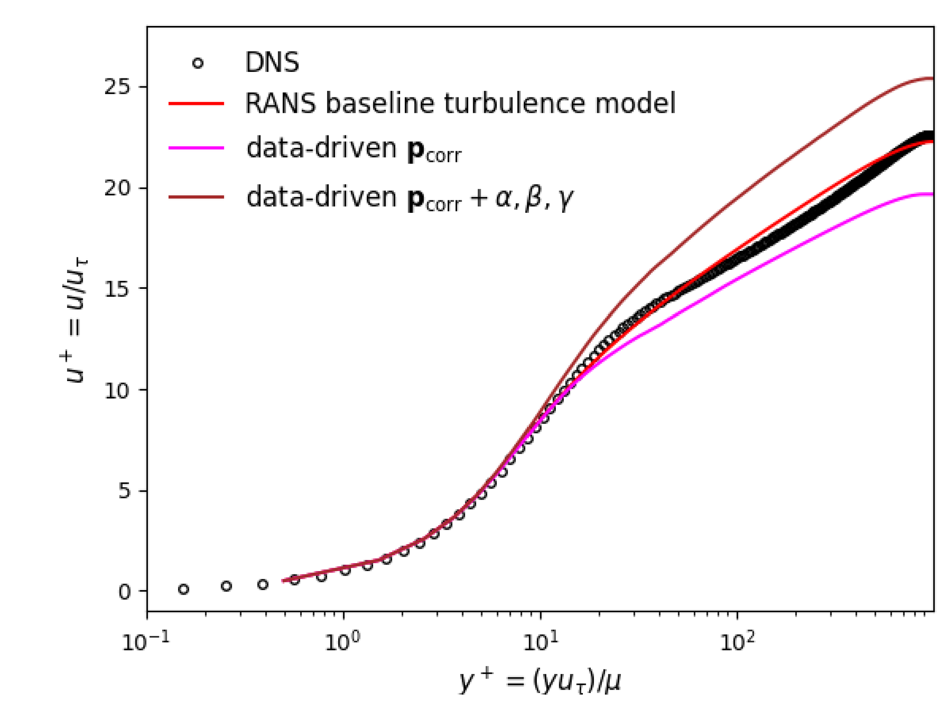
Physics-informed augmented turbulence model

Turbulent channel flow

The random forest model, predicting the perturbation direction vector $\mathbf{p}_{\mathrm{corr}}$, led to more accurate eigenvalues of the Reynolds stress tensor in the forward CFD-simulation (not shown here). A combination of propagating true eigenvalues and eigenvectors ($\mathbf{p}_{\mathrm{corr}} + \alpha, \beta, \gamma$) resulted in an improved prediction of the Reynolds stresses, although actually only the anisotropy tensor was corrected without modifying the turbulent kinetic energy explicitly. Therefore, the different behavior of the shear stress component is accountable for the misalignment of the velocity profile for the simulations containing a machine learned correction.



Model predicted Reynolds stress tensor components at turbulent channel flow at $Re_\tau \approx 1000$



Streamwise velocity profile of turbulent channel flow at $Re_\tau \approx 1000$

References

[1] Iaccarino et al. (2017). "Eigenspace perturbation for uncertainty estimation of single point turbulence closures." In: Physical Review Fluids. 2, 2017

[2] Ling et al. (2016). "Machine learning strategies for systems with invariance properties.". In: J. Comput. Phys., 318:22-35.

[3] Wang et al. (2018). "Physics-informed machine learning approach for augmenting turbulence models: A comporehensive framework". In : Physical Review Fluids. 3, 2018

[4] Lee and Moser (2015). "Direct numerical simulations of turbulent channel flow up to $Re_\tau \approx$ 5200." In: Journal of Fluid Mechanics.