Surrogate Modeling of Subgrid Turbulent Transport based on 3D Radiative Hydrodynamic Simulations of the Quiet Sun

Rimsha Hameed Syeda[1] Dustin J. Kempton[1] Viacheslav Sadykov[1] Irina Kitiashvili[2]

[1]*Georgia State University*
[2]*NASA Ames Research Center*

Introduction

Turbulent Transport: Plays a critical role in astrophysical plasmas, such as the solar interior, spanning multiple scales and challenging traditional modeling approaches.

Objective: Develop machine learning (ML) models—MLP and CNN—to predict subgrid Reynolds stress tensors from StellarBox 3D simulations of the solar atmosphere.

Benchmarking: Compare ML-driven models against physics-based Gradient and Smagorinsky approaches.

Dataset

Simulations:

- 3D Radiative Hydrodynamic simulations from Stellarbox code [6], utilized in [5].
- Resolution: Horizontal 12.5 km; The domain spans 1 Mm above the photosphere and has 5.4 Mm of the convection zone and 2 hours of simulations are considered.

Data Preparation:

- **Step 1:** Consider the simulation output with a cadence of 5 minutes and divide 512×512×512 simulation cubes into non-overlapping 12×12×12 cells (50 km resolution).
- **Step 2:** Each 12×12×12 cell split into 27 smaller 4×4×4 sub-cells. Compute τ_{ij} for central sub-cell; average velocities/densities for all.
- **Step 3:** Generate one data point per 12×12×12 cell with features (velocities, density) and targets (τ_{ij}).

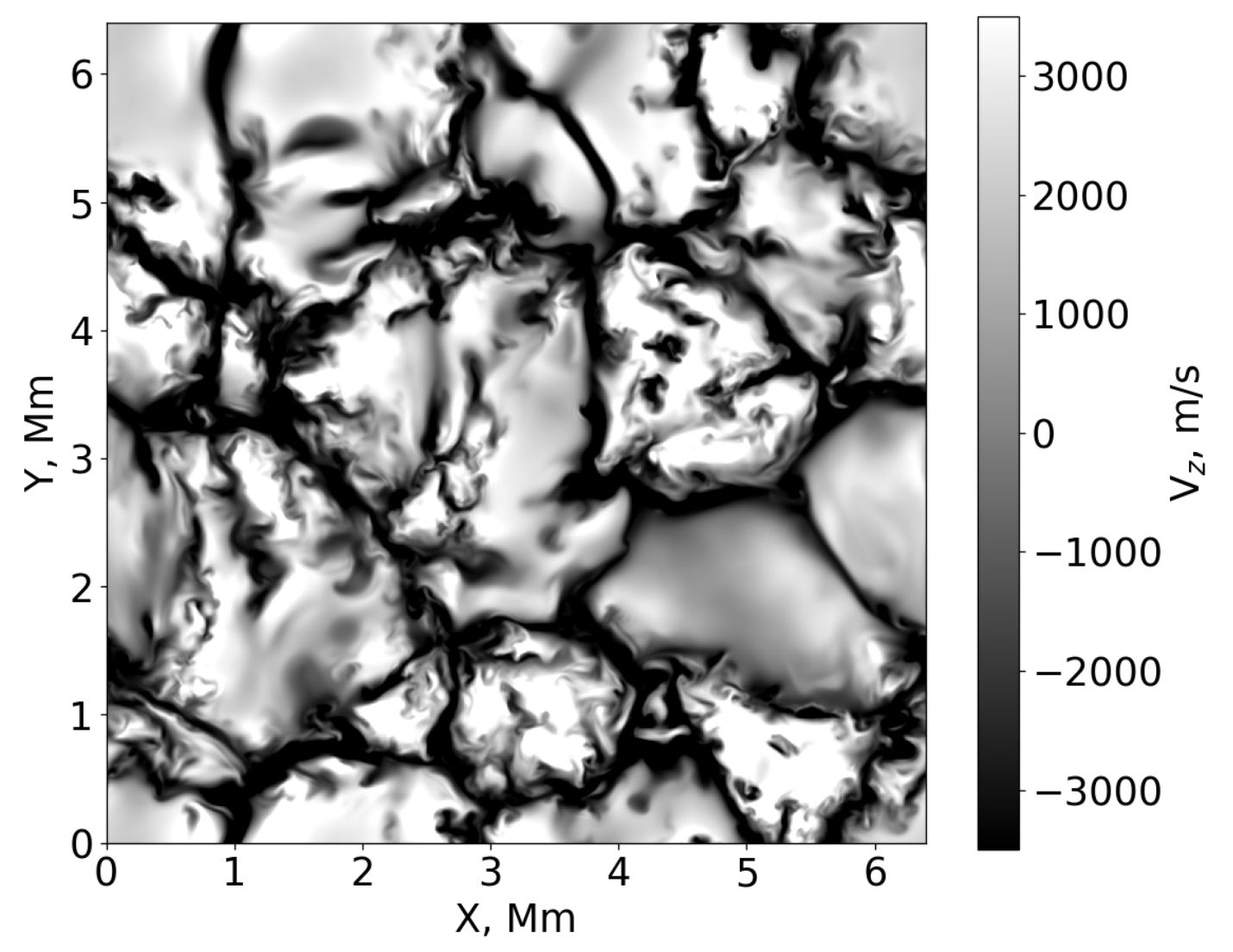
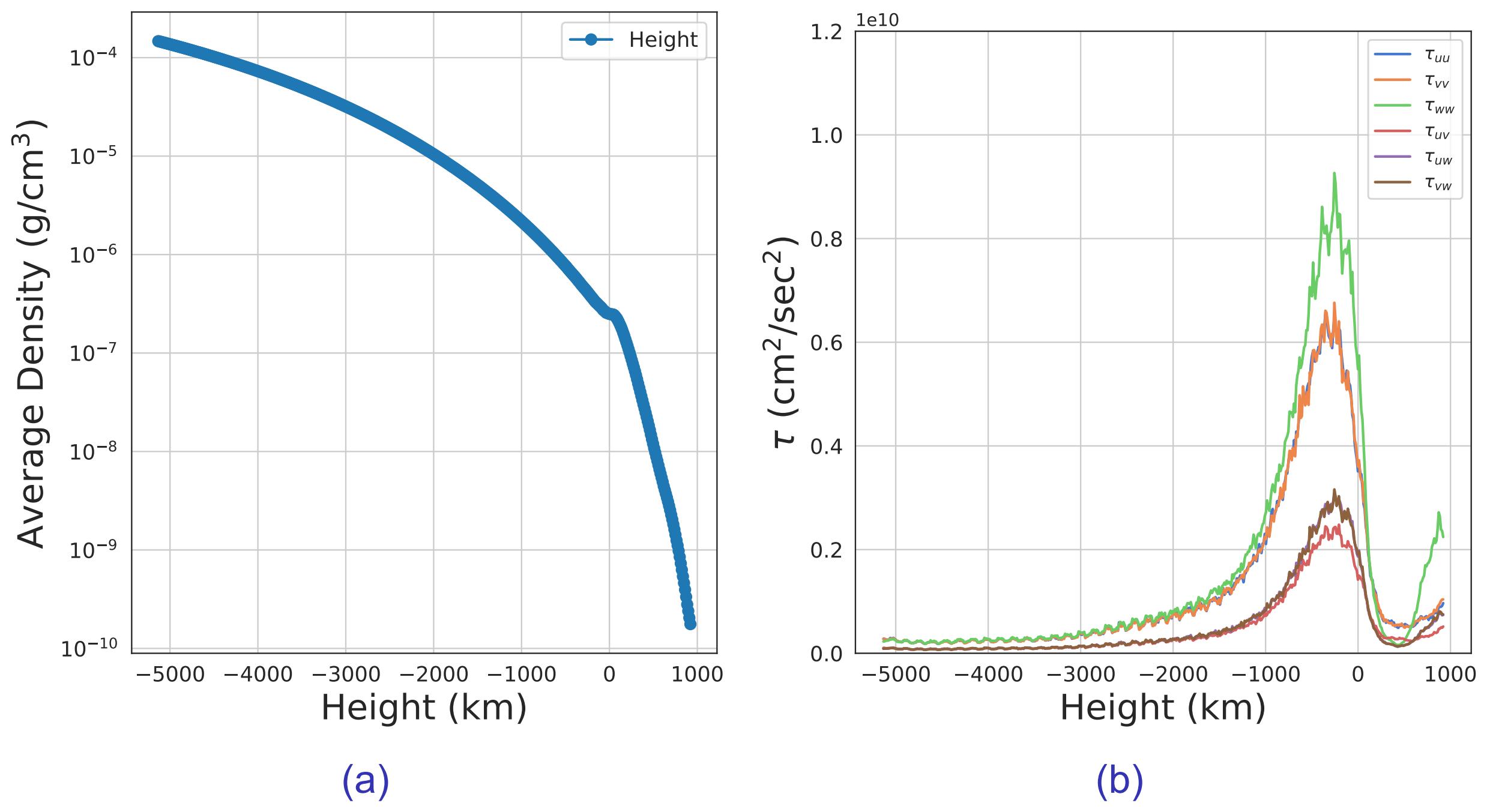


Figure 1. Vertical velocity at the $h = 0$ km for the first datacube of considered StellarBox simulations

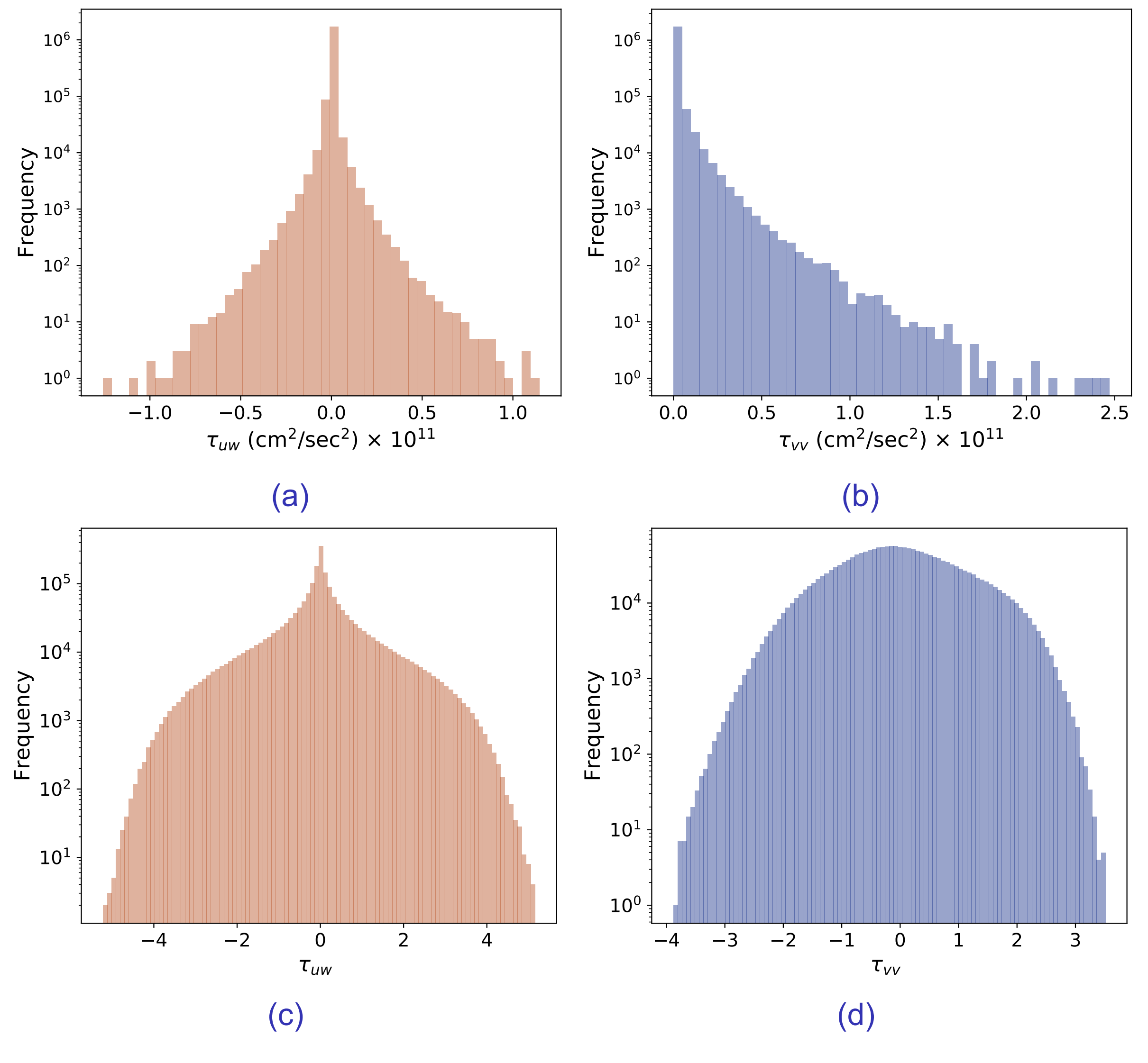


(a) (b)

Figure 2. (a) The distribution of average density as a function of height across the datacubes; (b) The distribution of the unsigned averages of all components of the Reynolds's Stress Tensor with respect to height across all data cubes.

Preprocessing:

- Velocity components: Standardized using 'StandardScaler'.
- Density: Logarithmic transformation to address skewness.
- Stress Tensor τ_{ij}: Logarithmic (diagonal terms), signed-logarithmic (off-diagonal terms).



(a) (b)

(c) (d)

Figure 3. (a) and (b) show the original distribution of τ_{uw} and τ_{vv}, (c) and (d) represent the transformed distributions of τ_{uw} and τ_{vv} after preprocessing, respectively

Methodology

Goal: Predict subgrid Reynolds stress tensor components (τ_{ij}) which are defined as:

$$\tau_{ij} = \widetilde{v_i v_j} - \tilde{v}_i \tilde{v}_j \tag{1}$$

Where v_i is the i-th component of the velocity, and $\tilde{}$ indicates the averaged value of the variable over the spatial scale of interest.

Baseline Models:

- **Gradient Model:** Uses a physics-based approach [2] to compute τ_{ij} from velocity gradients:

$$\tau_{ij} = \frac{\widetilde{\Delta}^2}{12} \partial_k \widetilde{u_i} \partial_k \widetilde{u_j} \tag{2}$$

- **Smagorinsky Model:** Originally introduced in [4], the aforementioned model approximates the subgrid stress tensor following [6]:

$$\tau_{ij} = -\frac{\Pi_{ij}}{\widetilde{\rho}} = -2\mu'_T \left(S_{ij} - \frac{1}{3} \partial_k \widetilde{u_k} \delta_{ij} \right) + k'_T \delta_{ij} \tag{3}$$

$$\mu'_T = \widetilde{\Delta}^2 \left(C_S |S| + C_D |\partial_k \widetilde{u_k}| \right), \qquad k'_T = \frac{2}{3} C_C \widetilde{\Delta}^2 |S|^2 \tag{4}$$

$$S_{ij} = \frac{1}{2} \left(\partial_j \widetilde{u_i} + \partial_i \widetilde{u_j} \right), \qquad |S| = \sqrt{2 S_{ij} S_{ij}} \tag{5}$$

Smagorinsky model has two coefficients C_C and C_S, as well as a shock-capturing coefficient C_D. In this work, we utilize $C_S = C_C = 0.1$, and $C_D = 0$ as mentioned in [1].

ML Models:

- **1. MLPRegressor:** A fully connected neural network scikit-learn [3] with two hidden layers optimized using GridSearchCV.
- **2. Convolutional Neural Networks:**
  3DCNN1: Velocity components are convolved to extract spatial features, while scalar density is introduced after convolutional operations. Outputs are concatenated before fully connected layers.

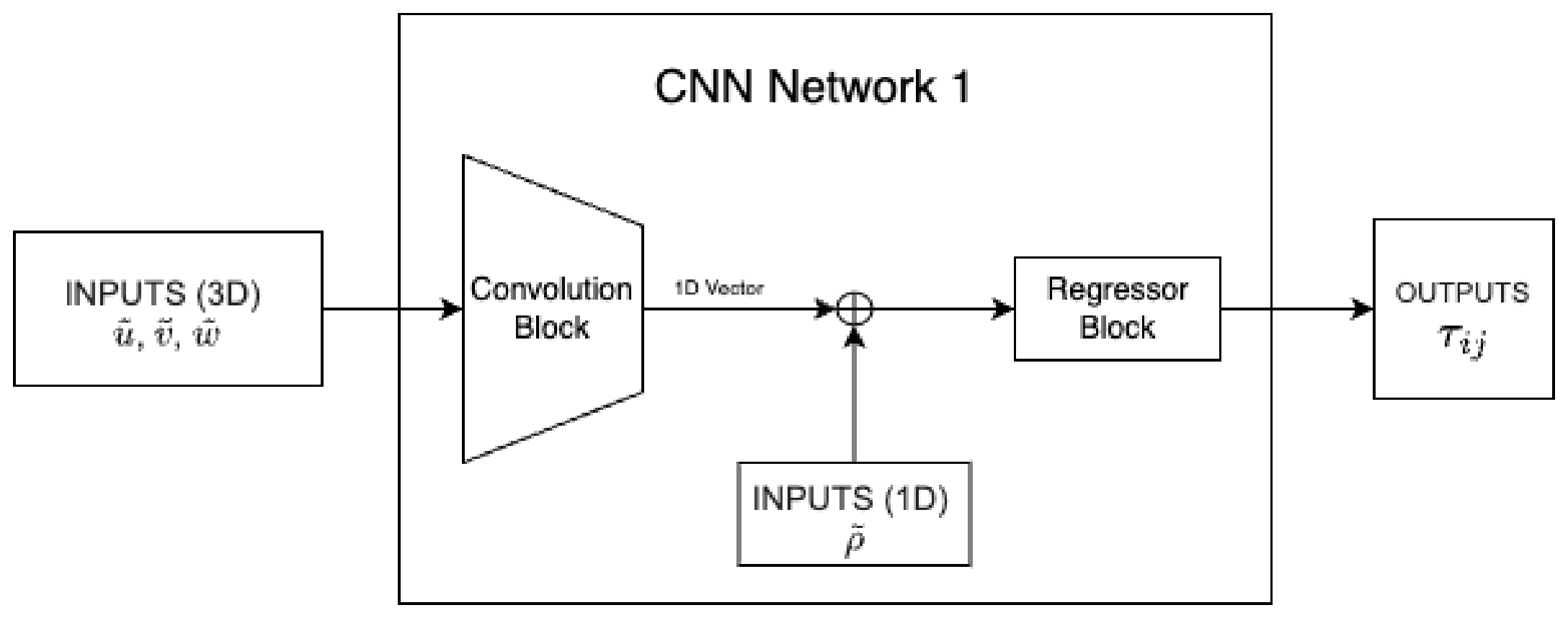


Figure 4. Model Schematics of 3DCNN

Experimental Settings

Selected Model Settings:

MLP Tuning We optimized MLP hyperparameters using GridSearchCV [3]. The best parameters chosen are given in Table 1.

Table 1. Model Settings.

Layers	Activation	Solver	Alpha	Learning Rate	Learning Init	Max Iterations
(100, 100)	Tanh	Adam	0.01	Adaptive	0.001	$1,000$

CNN Tuning Both the CNNs parameters were refined for stability and accuracy:

Learning Rate: 0.001 selected for stable training

Epochs: 50 with early stopping after 10 epochs with no improvement

Batch Size: 128 for balanced performance and speed

Activation: LeakyReLU (3DCNN1.1), Softsign in dense layers

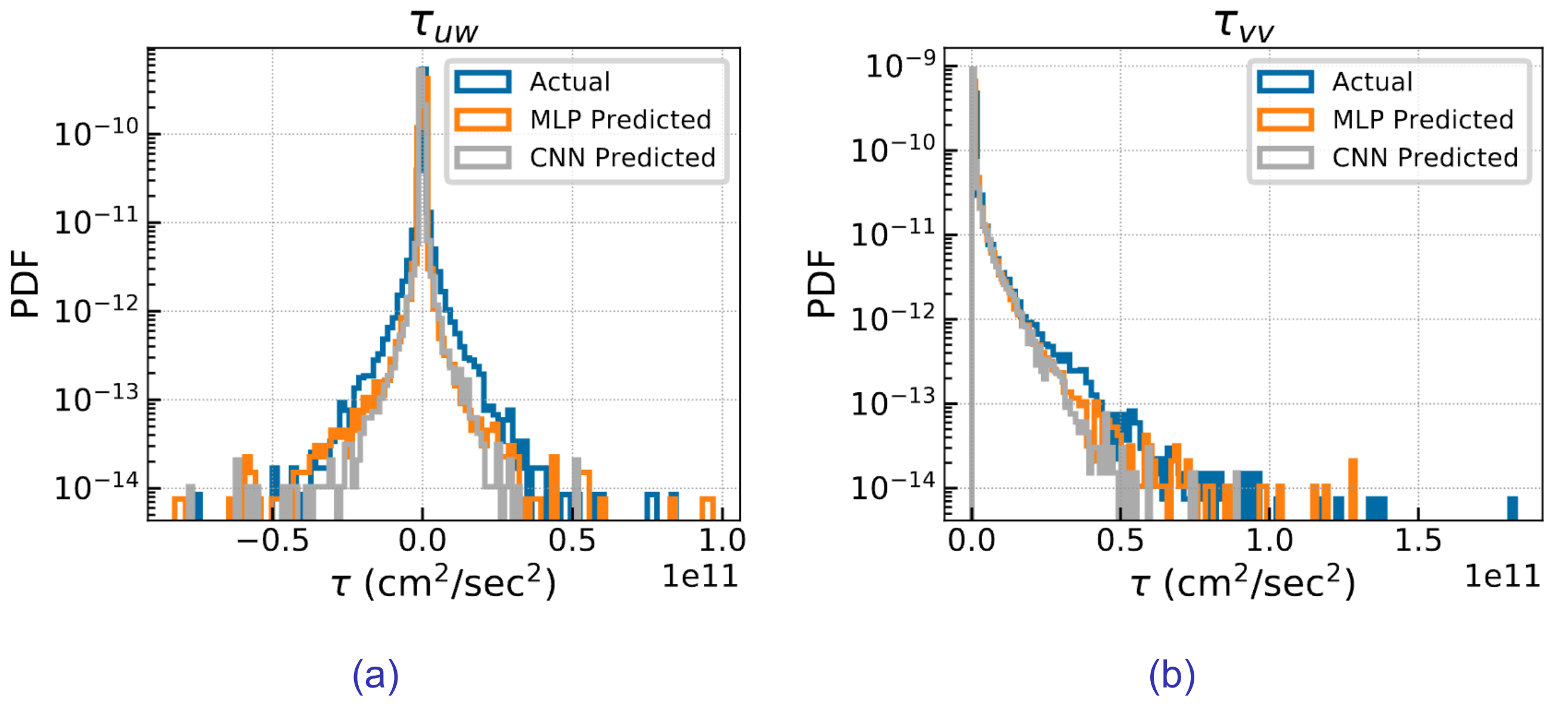
Optimizer: Adam

Architecture: 64 filters, kernel size 3

Outcome: Improved regression accuracy and model robustness in predicting turbulence.

Results

The optimized MLPRegressor and CNN performance was evaluated based on its ability to predict the subgrid Reynolds stress tensor components τ_{ij}. The figures and table below show their optimized performances. In Figure 6a we show the Probability Density function of the distribution of original and predicted values of components τ_{ww} and τ_{vv} using MLP Regressor and 3DCNN.



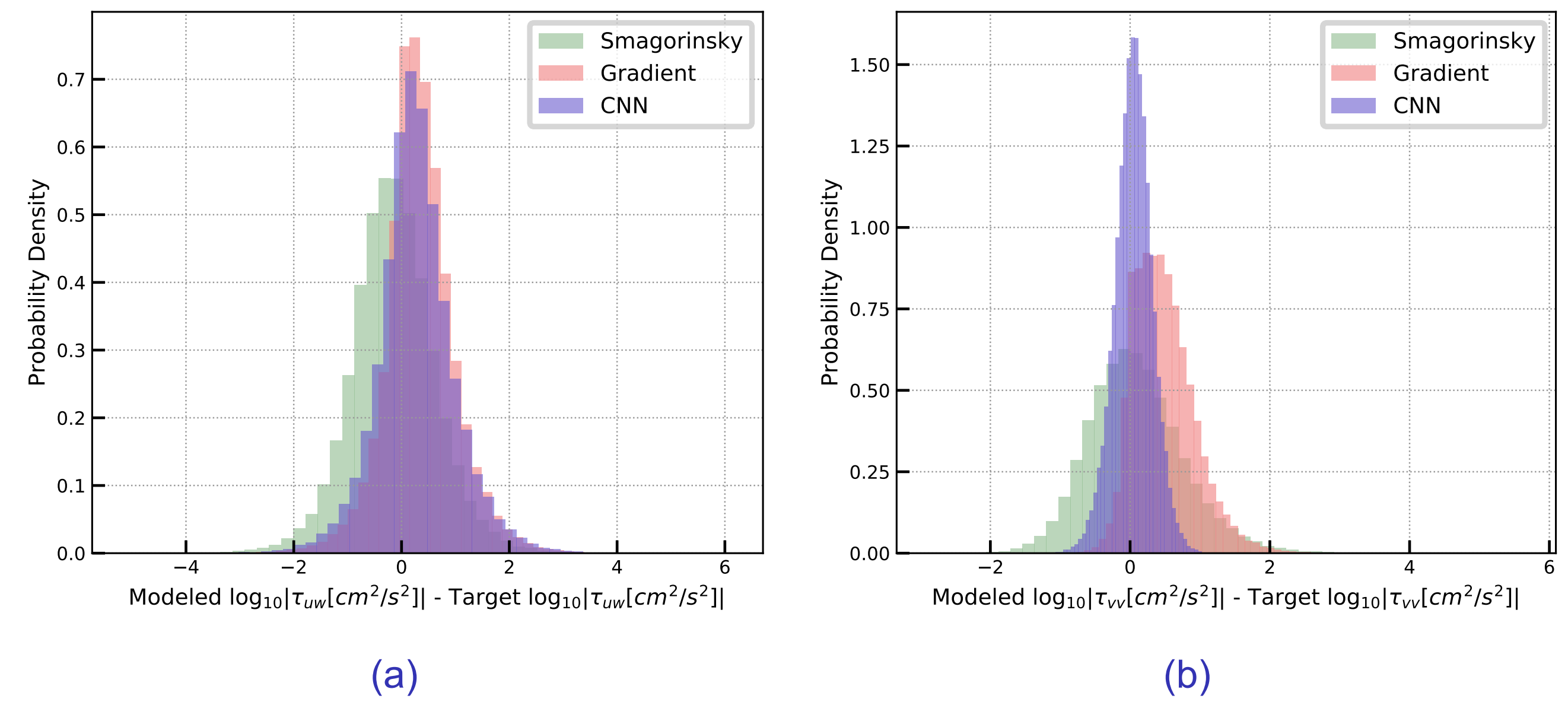
(a) (b)

Figure 5. PDF of components of τ. Blue shows the original target data, orange shows the predictions of the MLPRegressor, and grey shows the CNN predictions in subfigures (a) and (b)

In Table 2 we show the mean squared error for each of the stress tensor τ_{ij} target features across each model evaluated.

Table 2. MSE results in units of cm^2/s^2.

Method	τ_{uu}	τ_{uv}	τ_{uw}	τ_{vv}	τ_{vw}	τ_{ww}
Gradient	$3.53e+09$	$1.55e+09$	$1.81e+09$	$3.57e+09$	$1.83e+09$	$4.45e+09$
Smagorinsky	$3.71e+09$	$2.21e+09$	$2.56e+09$	$3.67e+09$	$2.57e+09$	$4.66e+09$
MLP	$2.82e+09$	$1.66e+09$	$1.86e+09$	$2.88e+09$	$2.18e+09$	$3.50e+09$
3DCNN1	$2.36e+09$	$1.42e+09$	$1.67e+09$	$2.50e+09$	$1.70e+09$	$3.13e+09$



(a) (b)

Figure 6. Comparison of the subgrid stress tensor components predicted by the Multi-Layer Perceptron (MLP) model, CNN Model, and physics-based Gradient and Smagorinsky models with the actual (target) values. in subfigures (a) and (b)

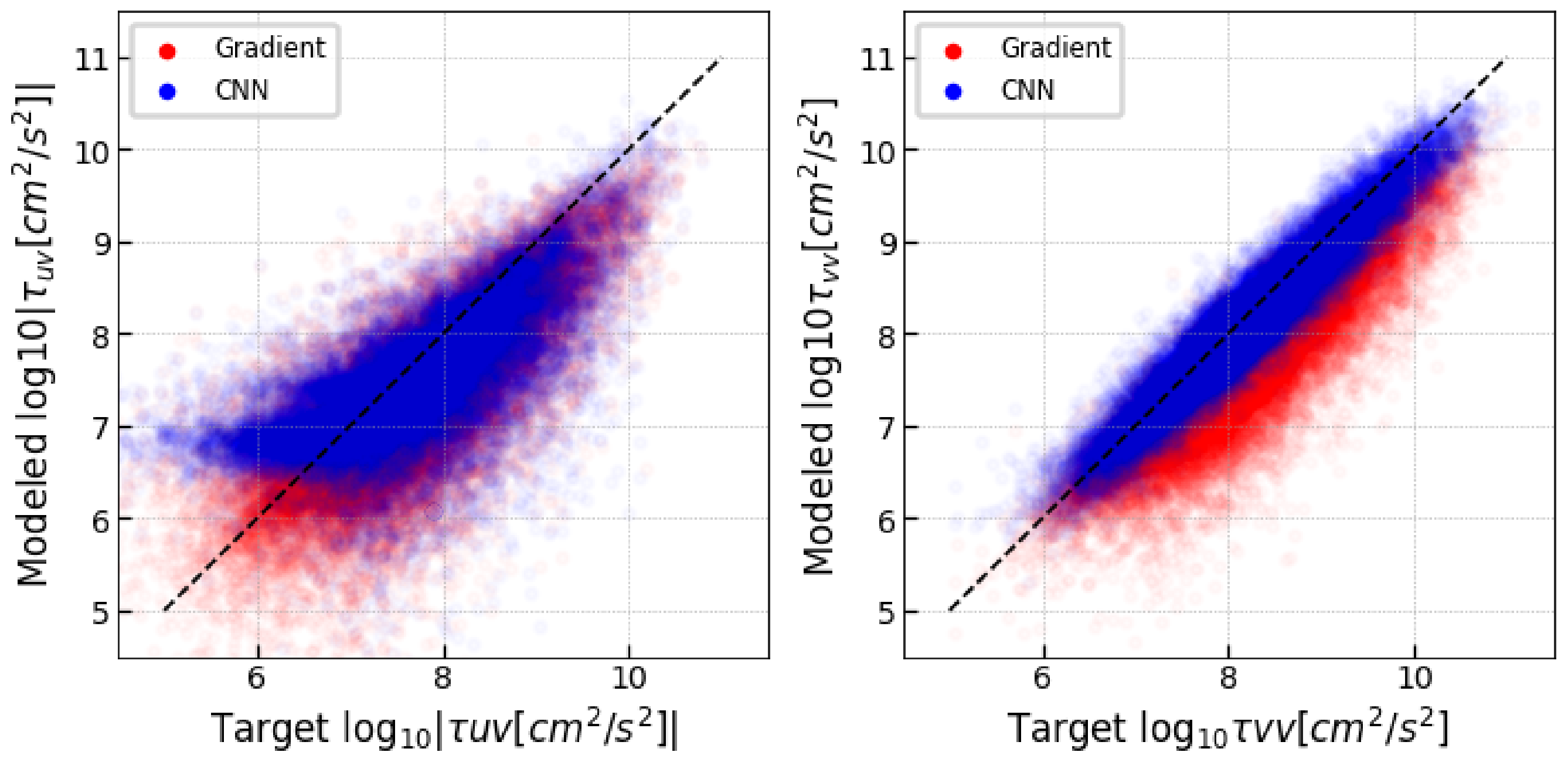


Figure 7. Comparison of the subgrid stress tensor components predicted by the CNN Model, and physics-based Gradient model with the actual values of the off-diagonal component(left) and diagonal component(right) of the target

Conclusion

- We developed a prototype of the ML-driven model using MLPRegreesor and CNN for predicting the subgrid Reynolds Stress Tensor components (τ_{ij}) for 3D realistic simulations of the Sun.
- The model targets the ∼50 km spatial resolution and is developed based on the high-resolution, 12.5 km, StellarBox simulations.
- Conducted extensive experimentation and parameter tuning on the MLPRegressor and CNN models, gaining insights into the model's architecture and hyperparameters' impact on performance.
- This demonstrated the effectiveness of the CNN in capturing complex relationships within the data.
- Results demonstrate better performance of machine learning models than baseline models (Gradient and Smagorinsky).
- Future work: generalization techniques like weighted loss function which can help reduce overfitting and enhance the model's ability to capture both high and low-probability regions,

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