Oral presentation | Turbulent flow

Turbulent flow-I

Tue. Jul 16, 2024 4:30 PM - 6:30 PM Room B

[6-B-01] *A priori* test of a data-driven SGS model considering the multiscale nature of turbulent flows

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A priori test of a data-driven SGS model considering the multiscale nature of turbulent flows

<u>Bahrul Jalaali</u> and Kie Okabayashi Department of Mechanical Engineering Osaka University



Outline

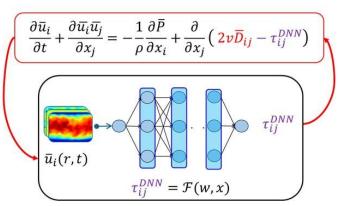
Background & Objective

- II. Analysis object & problem setting
- III. Preparation of training dataset
- IV. Framework of data-driven turbulence model
- V. Target for comparison
- VI. Result of a priori test
- VII. Conclusion



Concept of Data-driven SGS model Department of Mechanical Engineering

- In recent years, many attempts have been reported to construct data-driven sub-grid scale (SGS) models with deep neural networks (DNN).
- Unlike conventional models, data-driven SGS models are expected to inductively extract subfilter-scale fluctuations and create phenomenon-based models that do not contain artificial approximations or assumptions when trained in appropriate settings.



 \hat{y} : output/prediction x: input data

 \mathcal{F} : model

r, t: position and time

w: weight

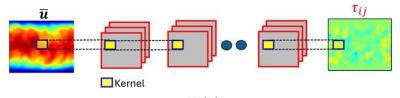
Duraissamy et al. (2019). Annu. Rev. Fluid Mech.

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Related work

- Data driven SGS model has been deployed based on local approach of multilayer perceptron (MLP)^{1,2} and non-local approach of convolutional neural network (CNN) approach² showing a good result in predicting residual stress 3,4
- DNN architecture is critical in data driven SGS model since it involve a large range of different scales of eddies



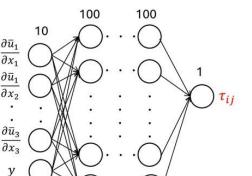
 $\tau_{ij} = \mathcal{F}(\overline{u})$

Data driven SGS based on CNN

Gamahara, M, Hattori, Y. (2017). Physical review fluids 3. Liu et. al. (2022) AIP Advances Park, J and Choi H. (2021). J. Fluid mech.

4. Saura, N and Gomez, T. (2023). EPL

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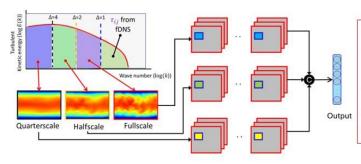
 $\tau_{ij} = \mathcal{F}(\nabla \overline{u}, y)$

Data driven SGS based on MLP

Multi-scale CNN-based SGS model Graduate School of Engineering Department of Mechanical Engineering



- Multi-scale nature of turbulence vortices → involve a range of vortices scale
- The multi-scale CNN is separating the input to several representation focusing on different scale and progressively encode information from coarser to the finest scale.



Objective

To investigate whether the new multi-scale CNN model can extract features of turbulence vortices of various scales and how the algorithm affects the prediction accuracy of the residual stresses.

Illaramendi, et. al. (2022). Data centric engineering
 Fukami, et. al. (2020). Theor. Comput. Fluid Dyn.

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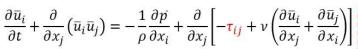


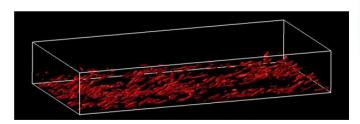


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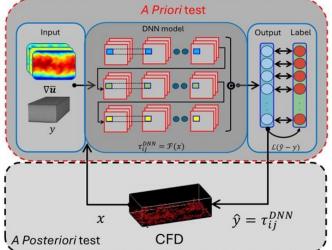
Analysis object & problem setting







Channel turbulence friction Reynolds number ($Re_{ au}=u_{ au}\delta/
u$) 180



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Dataset preparation: DNS data

Governing Equation

$$\frac{\partial u_i}{\partial x_i} = 0 \ ; \\ \frac{\partial u_i}{\partial t} + u_j \\ \frac{\partial u_i}{\partial x_j} = \delta_{i1} \\ - \frac{\partial p}{\partial x_i} \\ + \frac{1}{Re_\tau} \\ \frac{\partial^2 u_i}{\partial x_i x_j}$$

Reynolds number ($Re_{\tau}=u_{\tau}\delta/\nu$): 180

Computational setup

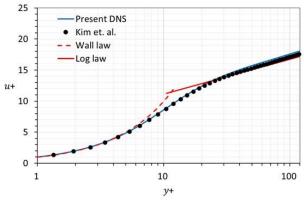
Grid arrangement: collocated grid Time marching: 2nd-order Adams-Bashforth method Convection & viscous terms: 2nd-order central difference Coupling of u & p: fractional step method

. .

Computational domain

Variable	Value			
$L_x/\delta \times L_y/\delta \times L_z/\delta$	$4\pi \times 2 \times 2\pi$			
$\Delta x^+ \times \Delta y_{\max}^+ \times \Delta z^+$	$11.8 \times 5.4 \times 7.1$			
$N_x \times N_y \times N_z$	$192\times128\times160$			

 $L_{y} = 2\delta$ V $L_{y} = 2\delta$ L_{y} L_{y}



1. Okabayashi, K. (2016). Journal of Fluid Science and Technology 2. Kim et. al. (1987). Journal of Fluid Mechanics

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Dataset preparation: Filtering

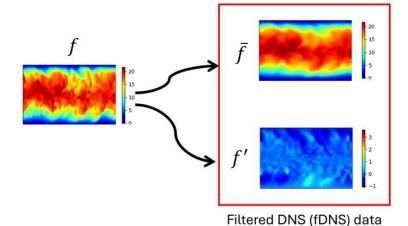
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- The dataset for training DNN model is obtained from high fidelity DNS data through filtering process.
- Filtering process will decompose the grid-scale (\bar{f}) and subgrid-scale (f') components that match the LES grid. The box filter

$$G(x) = \begin{cases} 1/\Delta & (|x| < \Delta/2) \\ 0 & (|x| > \Delta/2) \end{cases}$$

is used.

Δ: filter size



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Wang, et. al (2018). Physics of fluid Wu, et. al. (2018). Physical review fluids Gamahara,M, Hattori, Y. (2017). Physical review fluids Prakash et. al. (2022). Comput. Methods. Appl. Mech. Engrg.

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The choice of input and output features

• It can be assumed that residual stress may be written as a functional strain and rotation rate tensor as:

$$\tau_{ij}^{DNN} = \mathcal{F}\left(\overline{D}_{ij}, \overline{\Omega}_{ij}\right).$$

- Previous studies 1,2,3,4 found that $\frac{\partial \overline{u}_i}{\partial x_i}$ is the most influential variable rather than \overline{D}_{ij} and $\overline{\Omega}_{i,i}$.
- Including $\frac{\partial \overline{u}_i}{\partial x_i}$ as an input, the data-driven SGS model will satisfy Galilean invariance.
- The scalar value of distance from the wall information (y) is provided to give model robustness. Therefore, the data driven SGS model is defined as

$$\tau_{ij}^{DNN} = \mathcal{F}\left(\frac{\partial \bar{u}_i}{\partial x_j}, y\right)$$

 $\frac{\partial \overline{u}_i}{\partial x_i}$: Velocity gradient tensor

• Label data is obtained as $au_{ij} = \overline{u_i u_j} - \overline{u_i} \overline{u_j}$.

 \overline{D}_{ij} : Rate-of-strain tensor $\overline{\Omega}_{ij}$: Rotational rate tensor

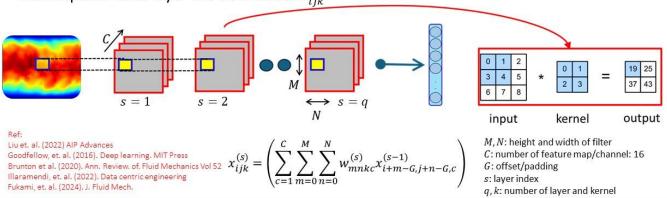
Convolutional neural network (CNN) Graduate School of Engineering

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- CNN algorithm is chosen since it provides the advantages of extracting features while preserving location information \rightarrow provides robustness against spatial invariance.
- To deal with interaction between multiscale phenomena on 3D turbulent flow, 3D CNN algorithm is employed

• The output of each layer are defined as: $x_{ijk}^{(s)}$

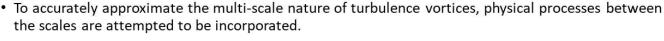


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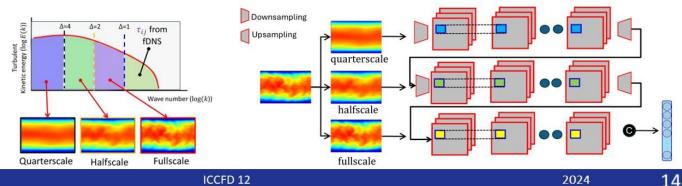
Illaramendi, et. al. (2022). Data centric engineering Fukami, et. al. (2024). J. Fluid Mech

Multi-scale CNN

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 The input variable will be down-sampled into half and quarter size in which similar with filtering operation. The quarter-scale focuses on largest eddies scale which is the dominant feature while the full-scale retain all eddies scale information. The information from coarsest scale to the finest scale will be progressively encoded ensuring the transfer energy process. The resulting output of each process is concatenated in the final layer



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Loss function (1)

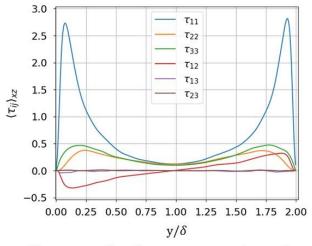
• The loss function consist of data-based loss (\mathcal{L}_d) , physics constrained loss (\mathcal{L}_p) , and regularization loss (\mathcal{L}_r) .

$$\mathcal{L} = \mathcal{L}_d + \mathcal{L}_p + \mathcal{L}_r$$

- The average value of τ_{13} and τ_{23} are very low, making the nonlinear regression of DNN model hard to be reconstructed.
- The constant β is introduced to magnify the influence of τ_{13} and τ_{23} . Therefore, \mathcal{L}_d is described as:

$$\mathcal{L}_d = \sum_{j=1}^6 \left(\frac{\beta_j}{N} \sum_{i=1}^N (y_i - \widehat{y_i}) \right)$$

 y_i : label/truth data (τ_{ij}) \hat{y} : output/predicted data



The average value of au_{ij} over stream and spanwise direction w.r.t channel height

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Ref: Goodfellow, et. al. (2016). Deep learning. MIT Press Raissi et al. (2019). J. Comput. Phys., 378:686–707 Bose, R., Roy., A. (2024). Engineering Applications of Artificial Intelligence 128

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Loss function (2)

- To satisfy the physical condition, physics constraint loss function (\mathcal{L}_p) is introduced by adding the physical data of filtered velocity.
- Regularization loss (\mathcal{L}_r) is applied to avoid overfitting. Thus, the total loss function is defined as:

$$\begin{split} \mathcal{L} &= \mathcal{L}_d + \mathcal{L}_p + \mathcal{L}_r \\ \mathcal{L} &= \sum_{j=1}^6 \left(\frac{\beta_j}{N} \sum_{i=1}^N (y_i - \widehat{y_i}) \right) + \sum_{j=1}^6 \left(\frac{1}{N} \sum_{i=1}^N \Theta(y_{2i} - \widehat{y_i}) \right) + \lambda \frac{1}{N} \sum_{i=1}^N w_i^2 \end{split}$$

 y_{2i} is calculate from fDNS data, denote as $y_{2i}=\overline{u_iu_j}-\overline{u_i}\overline{u_j}$ Whereby in the calculation, the data of velocities will be embedded, not τ_{ij} \mathcal{L}_d : Loss data-based \mathcal{L}_p : Loss physics-based \mathcal{L}_r : Loss regularization w: weight x: input β , θ : constant y_i : label/truth data (τ_{ij}) \hat{y} : output/predicted data

 λ : regularization constant

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Outline

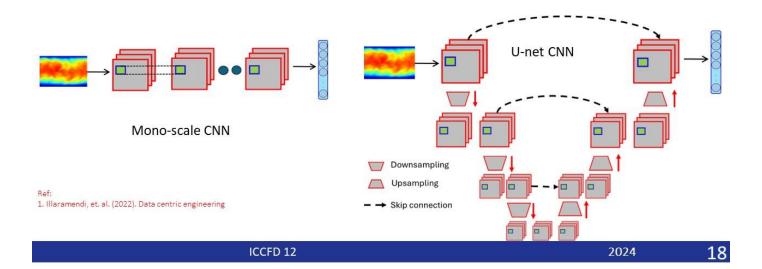
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Architecture comparison



• To investigate the performance of multiscale model, the comparison between the conventional CNN ("mono-scale CNN") and U-net¹ is carried out.





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Ref: Gholamy, A., et. al. (2018) Why 70/30 or 80/20 Relation between Training and Testing Sets: A Pedagogical Explanation. Departmental Technical Reports (CS)



Training and test

- Dataset for training and test
 - Input data: field of $\frac{\partial \overline{u}_i}{\partial x_i}$, y (distance from walls)
 - Label data: field of $au_{ij}=\overline{u_iu_j}-\overline{u}_i\overline{u_j}$
 - Amount of input: 10,000 instantaneous fDNS data (out of $0 \le t \le 120$). 8,000 for training data and 2,000 for test data.
- Correlation coefficient

$$CC[\tau_{ij}^{fDNS},\tau_{ij}^{p}] = \frac{\langle (\tau_{ij}^{fDNS} - \langle \tau_{ij}^{fDNS} \rangle)(\tau_{ij}^{p} - \langle \tau_{ij}^{p} \rangle) \rangle}{\sqrt{\langle ((\tau_{ij}^{fDNS} - \langle \tau_{ij}^{fDNS} \rangle)^{2} \rangle}} \sqrt{\langle ((\tau_{ij}^{p} - \langle \tau_{ij}^{p} \rangle)^{2} \rangle}} \\ \frac{\tau_{ij}^{p} : \text{Predicted data}}{\langle . \rangle : \text{domain average}}$$

Correlation coefficient (1)



- High correlation value (averaged in the : spanwise, streamwise, and wall normal direction) implies successful learning.
- Multi-scale CNN provided most successful as CC value exceeds 0.8 for all τ_{ij} component.
- In mono-scale CNN, CC < 0.8 on au_{22} and au_{23} component while only au_{11} and au_{12} component are yielded CC > 0.8 for U-net.
- This result provides that multi-scale CNN predicts the residual stress more accurate than other models.

$\mathrm{CC}[au_{ij}^{fDNS}, au_{ij}^{p}]$	$ au_{11}$	$ au_{22}$	$ au_{33}$	$ au_{12}$	$ au_{13}$	$ au_{23}$	CC average
Multi-scale CNN	0.931	0.860	0.886	0.913	0.881	0.803	0.879
Mono-scale CNN	0.900	0.793	0.842	0.867	0.832	0.723	0.826
U-net	0.869	0.756	0.797	0.822	0.776	0.659	0.780

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Correlation coefficient (2)

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- τ_{11} is the easiest component to resolve as it given higher CC value for all model.
- The difficulties to resolve τ_{13} and τ_{23} are noted on Refs.^{1,2,3}. By applying present loss function, it helps the DNN model to effectively resolved τ_{13} and τ_{23} .
- Present result has a better CC value than Refs.^{1,2,3}, yielding that physical constrain loss function help the model to increase the correlation value.

$CC[au_{ij}^{\mathit{fDNS}}, au_{ij}^p]$	$ au_{11}$	τ ₂₂	$ au_{33}$	$ au_{12}$	$ au_{13}$	τ ₂₃	CC average
Multi-scale CNN	0.931	0.860	0.886	0.913	0.881	0.803	0.879
Mono-scale CNN	0.900	0.793	0.842	0.867	0.832	0.723	0.826
U-net	0.869	0.756	0.797	0.822	0.776	0.659	0.780

f^{DNS}: fDNS data $\tau_{i,i}^{p}$: predicted value

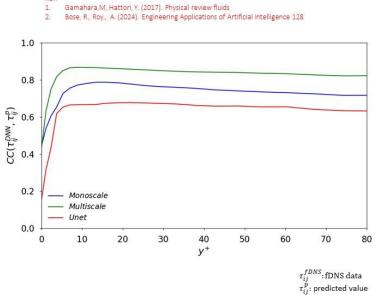
Gamahara,M, Hattori, Y. (2017). Physical review fluids Park, J and Choi H. (2021). J. Fluid mech.

Bose, R., Roy., A. (2024). Engineering Applications of Artificial Intelligence 128

Correlation coefficient (3)

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- The averaged CC value over span and streamwise w.r.t y⁺ is plotted.
- The result shows the superiority of multi-scale CNN on achieving better result than that of mono-scale CNN and U-net.
- In general, all models provide almost constant CC value on $y^+ > 5$. This constant result can be regarded as the ability of DNN model to effectively predict the residual stress in a whole domain and will not be degraded in specific region.

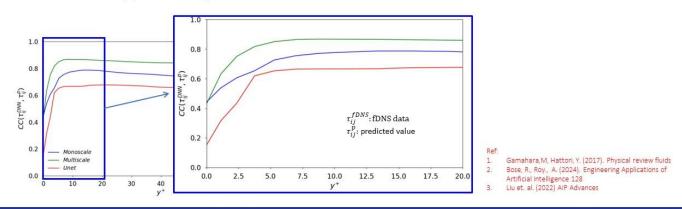


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Correlation coefficient (4)



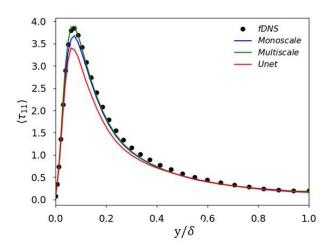
- On the viscous sublayer region, $y^+ < 5$, all model correlation was decreased especially near the wall.
- This results are in contrast with local approach of Refs. 1,2,3, meaning that local approach MLP has a better ability to predict near the wall since it maps the information locally. Meanwhile, non-local CNN approach is given more robust result on the whole domain.





Wall-normal distribution of au_{ij}

- The wall-normal distribution and the averaged τ_{ij} is investigated.
- The τ_{11} predicted from the multi-scale CNN is obviously closer to fDNS compared to the conventional mono-scale CNN and U-Net.
- By having higher average value, τ_{11} is considerably easier component to be learned by nonlinear regression model of data-driven model.

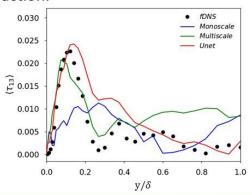


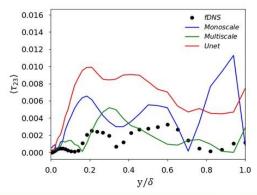
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Wall-normal distribution of au_{ij}



- Conversely, due to the small average value, au_{13} and au_{23} are difficult to approximate.
- Both mono-scale and U-net algorithms overpredict the τ_{13} and τ_{23} .
- Meanwhile, the multi-scale CNN has been successfully predicting those values adequately.
- This result showed that the ability of multi-scale on extracting small value or small scales interaction.



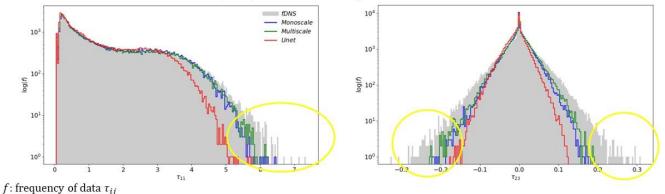


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Model performance on value distribution

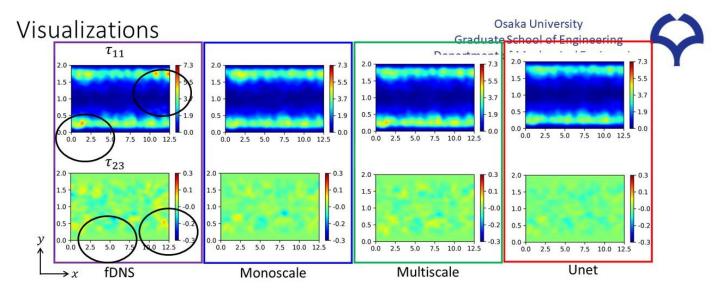
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The frequency distribution of the prediction and fDNS.



Overall, all models have been struggling to predict 'outliner' data shown on yellow circle, indicating the limitation of model. However, compared to mono-scale and U-net, multi-scale is considerably better as it can resolve τ_{11} and low value of τ_{23} adequately. It yielded that multi-scale is more effectively to capture and resolve the dynamics complexity of turbulent field

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Spatial distribution of au_{11} and au_{23} are depicted above. It shows that multi-scale can resolve residual stress accurately on high value of τ_{11} . On the low value of τ_{23} , multi-scale has slightly outperformed mono-scale and U-net. Both mono-scale and U-net show relatively similar result on au_{11} and struggle in au_{23}

Discussion



- The multi-scale model outperforms both the mono-scale and U-net models in resolving τ_{ij} , demonstrating superior capability in extracting important flow features.
- ullet This model is accurately constructing au_{ij} within different regions, including the viscous sublayer, viscous wall, and outer layer, indicating its robustness in capturing varied flow dynamics while maintaining high CC value
- The investigation of τ_{11} and τ_{23} describes the multi-scale model's proficiency in resolving both large and small scales, highlighting its effectiveness in capturing the complete spectrum of turbulent structures.

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Discussion



- The progressive encoding of features from coarser to finer scales facilitates
 the incorporation of the energy transfer process between scales,
 resembling the energy cascade mechanism in turbulent flows.
- This step is crucial as it ensures that the multi-scale model effectively captures the intricate details of energy distribution across scales.
- By extracting features from large, intermediate, and small eddies, the multi-scale model provides the DNN with comprehensive information, enabling it to construct accurate nonlinear regression models for resolving τ_{ij} .

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- The multi-scale model outperforms mono-scale and U-net models in resolving τ_{ij} , effectively extracting key flow features across the viscous sublayer, viscous wall, and outer layer regions.
- By progressively encoding features from coarser to finer scales, it captures the energy transfer process, akin to the energy cascade, ensuring comprehensive detail retention for accurate predicting residual stress.
- This approach enhances the model's ability to capture both large and small scales feature, demonstrating its proficiency in non-linear regression model of DNN.

Acknowledgment

- This work was partly achieved through the Research Proposal-based Use of the Large-scale Computer System at the Cybermedia Center, Osaka University.
- This work was financially supported by JSPS KAKENHI Grant No. JP22K03925 and a Grant from Beasiswa Pendidikan Indonesia (BPI)/ LPDP (the Indonesian Endowment Fund for Education, Ministry of Finance of Republic of Indonesia)

Thank you