Data-driven subgrid-scale modeling for wall-bounded turbulence

Jiaxi Zhao
joint with S. Arisaka, Q. Li, T. Hasama, N. Ikegaya, W. Wang
NUS & Kajima & KU

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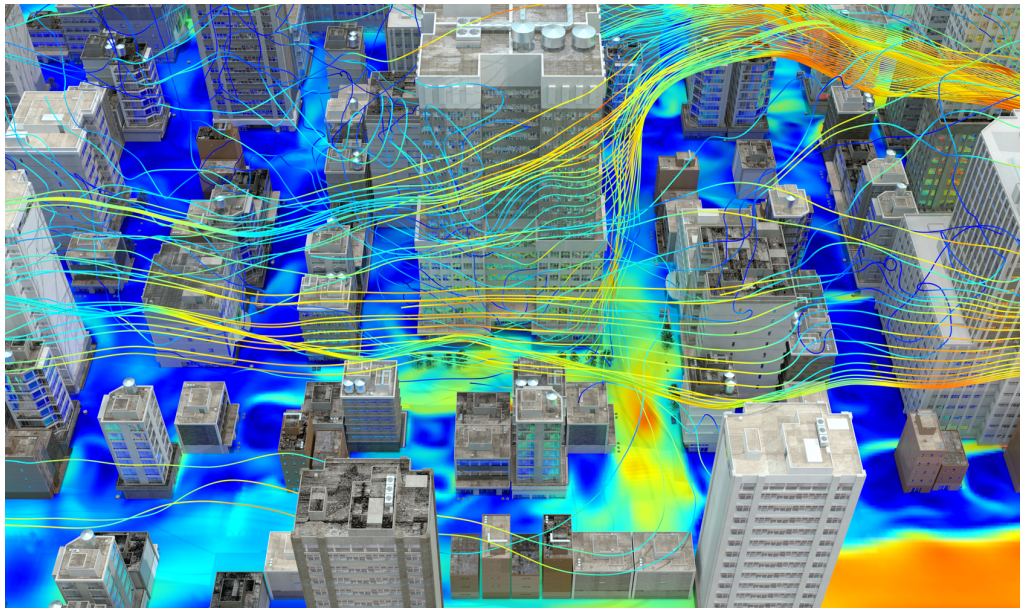
Motivation:

1. Performing DNS is unaffordable, even a LES with 50M grids of length 1000s takes several days.
2. Cheap simulation such as RANS and coarse-grid LES can not obtain accurate quantities such as peak pressure.



Can we design or learn better SGS models based on the LES data so that it can achieve accurate results even on coarse grid LES?

SGS stress modeling

There are three main issues for stress modeling:

1. The mapping from the input features. e.g. filtered velocity to the stress tensor is non-deterministic while most classical turbulence models and data-driven models are deterministic.

$$\overline{\mathbf{U}}, \nabla\overline{\mathbf{U}}, \overline{p} \overset{\text{NOT DETERMINISTIC}}{\Longrightarrow} \tau, \quad \min_{\phi} \left\| \tau - \phi(\overline{\mathbf{U}}) \right\|^2.$$

2. Discrepancy between a-priori error and a-posteriori error.

$$\left\| \widehat{\tau} - \tau \right\|^2, \quad \left\| \overline{\widehat{\mathbf{U}}}(T) - \overline{\mathbf{U}}(T) \right\|^2$$

3. Difficult to combine the OpenFOAM solver with gradient-based optimization algorithms.

Learning the SGS stress model

We test the following three approaches:

1. Directly predict the stress tensor from the input features.

$$\tau = \mathrm{NN}(\overline{\mathbf{U}}, \nabla\overline{\mathbf{U}}, \overline{p}). \tag{1}$$

2. Learn a correction of the constants to the Smagorinsky model.

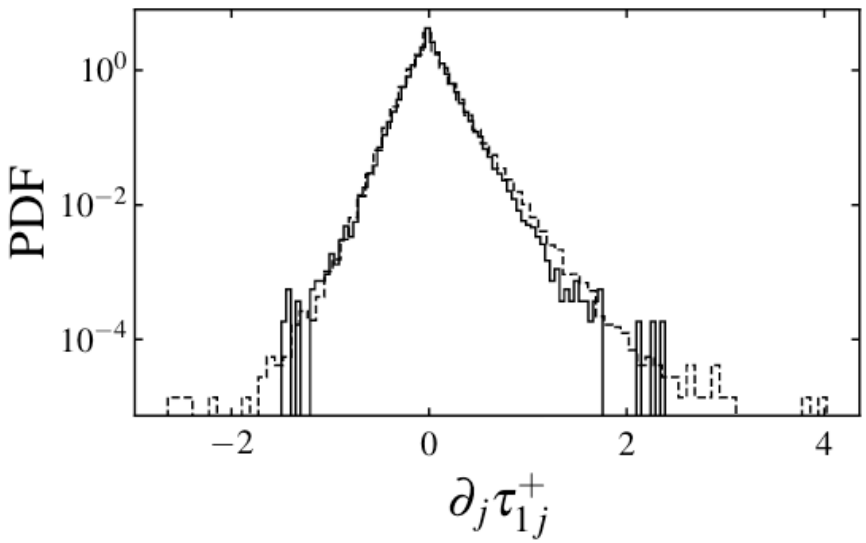
$$\widetilde{C} = \mathrm{NN}(\overline{\mathbf{U}}, \nabla\overline{\mathbf{U}}, \overline{p}) + C, \quad \nu_t = \widetilde{C}\Delta^2 \left|\bar{S}\right|. \tag{2}$$

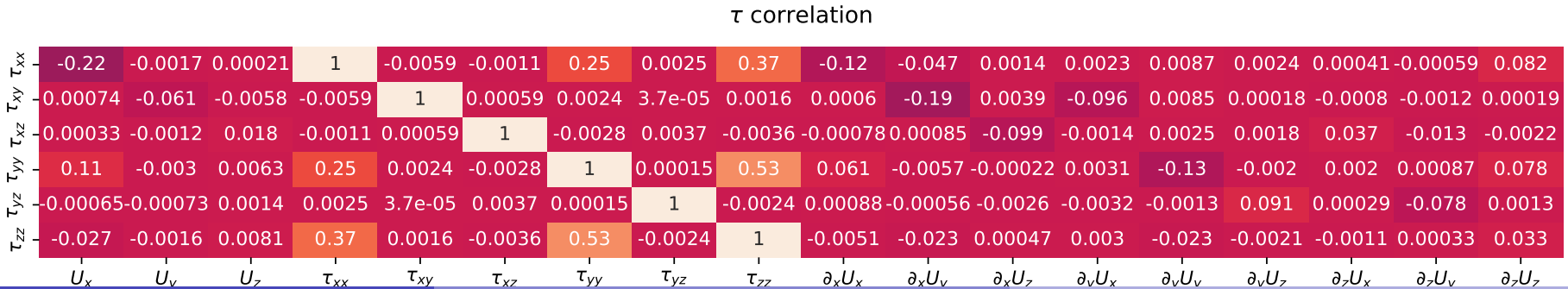
3. Learn a conditional generative model from the input features.

The first approach usually provides a much better a-priori error estimate than the second approach.

Probabilistic SGS stress modeling

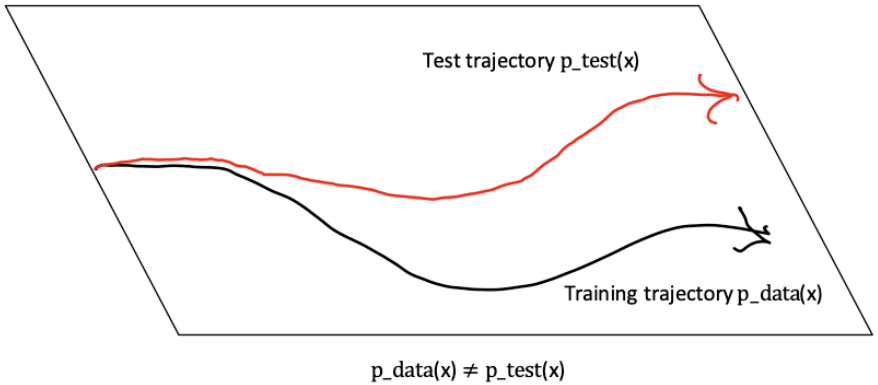
While the first two deterministic stress model can not capture the statistical behavior of the SGS stress, our probabilistic stress model manages this:





A-priori and a-posteriori discrepancy

The inconsistency between the a priori error and a posteriori error arises because the training algorithm does not take the solver dynamics into account.



The a-priori and a-posteriori performance are not consistent.

TABLE 3. Network and performance details

	Network inputs	Network outputs	*A priori* correlations	*A posteriori* simulations
NN-1	Local $\bar{S}_{ij}$	$\partial_j \tau_{ij}$	0.6	Stable; varying accuracy
NN-2	19-point stencil $\bar{S}_{ij}$	$\partial_j \tau_{ij}$	0.9	Unstable
NN-3	Local $\bar{S}_{ij}$	$L_i - D_i$ (Eq. 2.4)	0.7	Unstable

A toy case

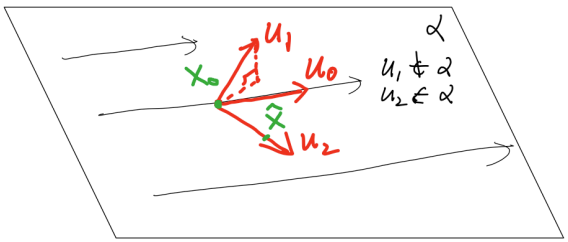
In a preliminary work, we apply tangent-space regularized method to solve the NS equation using the projection method.

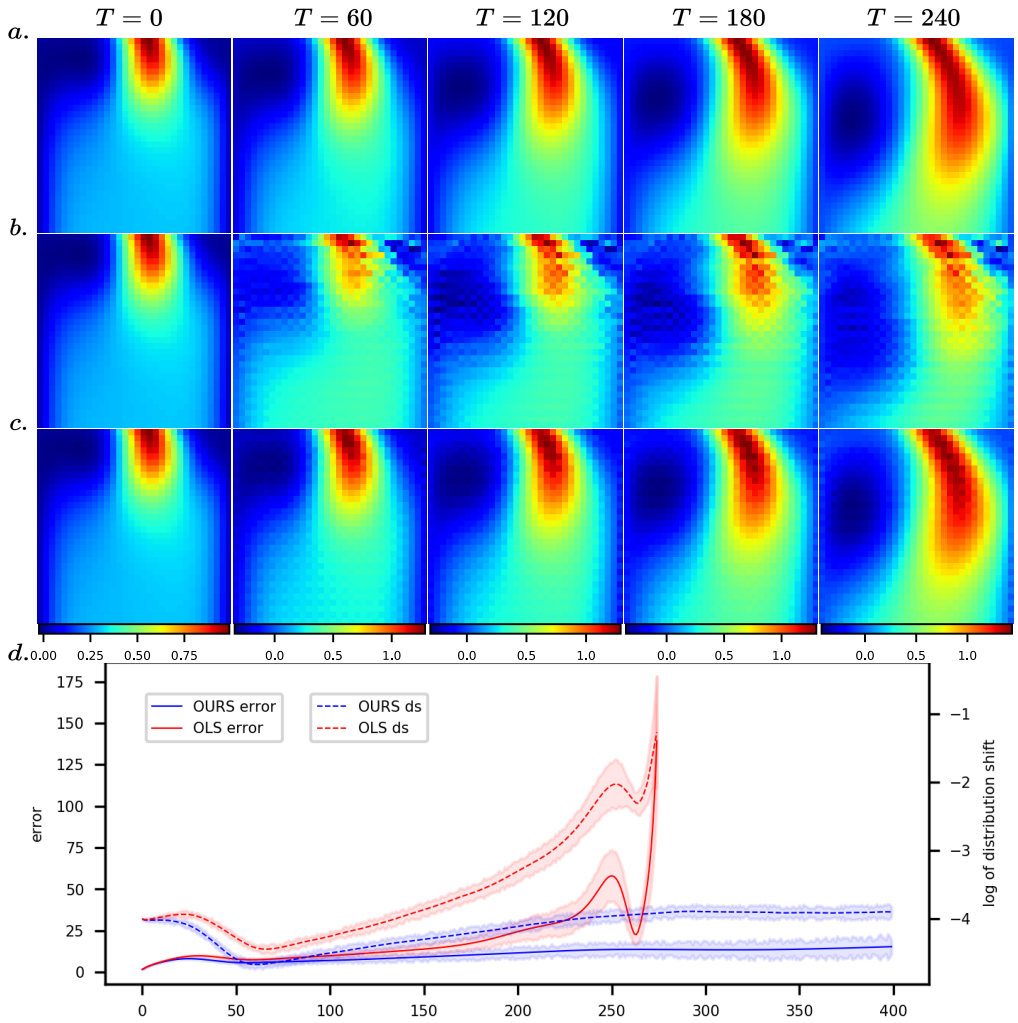
$$\mathbf{u}_{k+1} = \mathbf{u}_k + \Delta t(\nu \Delta \mathbf{u}_k - (\mathbf{u}_k \cdot \nabla)\mathbf{u}_k - \nabla p_k),$$
$$p_k = \phi(\mathbf{u}_k) = \Delta^{-1}(\nabla \cdot (\nu \Delta \mathbf{u}_k - (\mathbf{u}_k \cdot \nabla)\mathbf{u}_k)),$$

Instead of training the data-driven model to solely minimizing the a-priori error, we incorperate dynamical information, i.e. the iteration of the solver into the algorithm that accounts for a-posteriori error.

For fluid people, this part needs more time to explain, I skip most of the details this time.

A toy case[1]



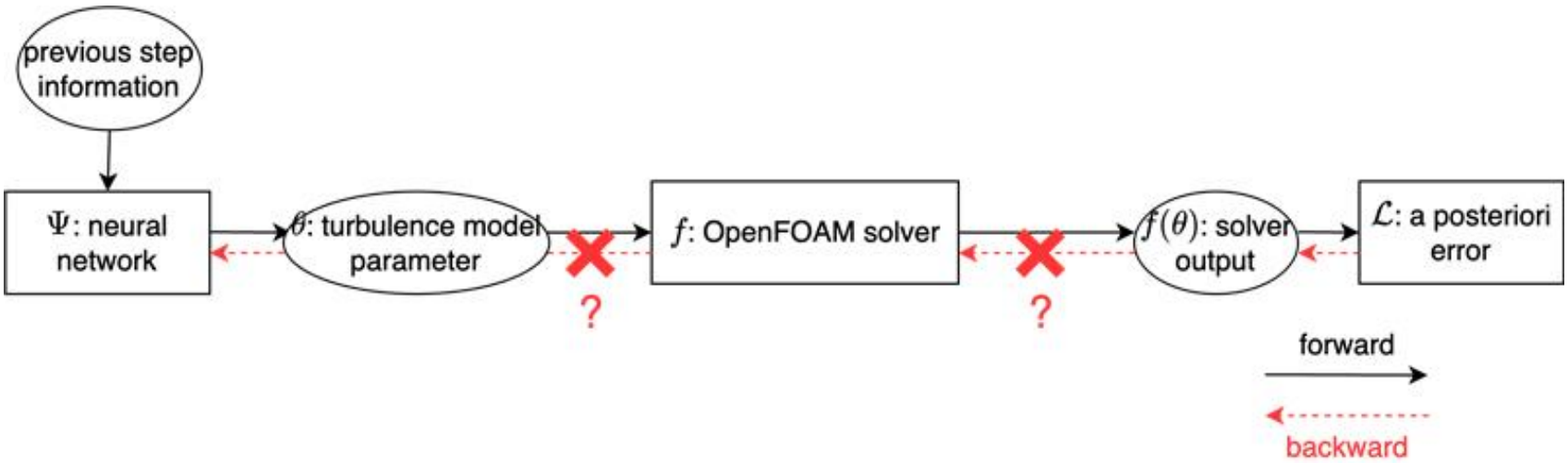


[1] J. Zhao and Q. Li (2024), Mitigating Distribution Shift in Machine Learning-augmented Hybrid Simulation, https://arxiv.org/pdf/2401.09259

Problem: Non-automatic-differentiable Solver

To directly minimize a posteriori error, we need to incorporate OpenFOAM solvers into the neural network training.

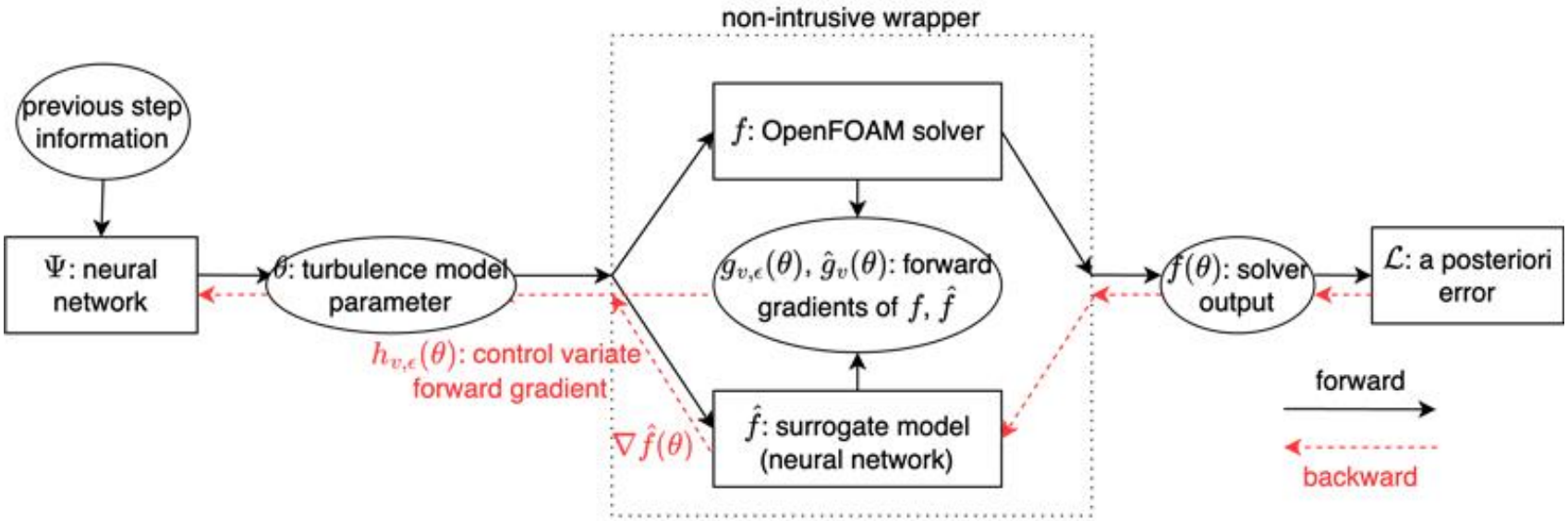
However, they are not automatic-differentiable, and computing gradients through them is not trivial.



Solution: Non-intrusive Wrapper

To enable joint training with neural networks and such solvers, we developed a non-intrusive methodolgy that wraps the solvers to be compatible with neural network training.

The key idea[2]is to construct an unbiased and low-variance gradient estimator using a surrogate model that mimics the solver behavior.

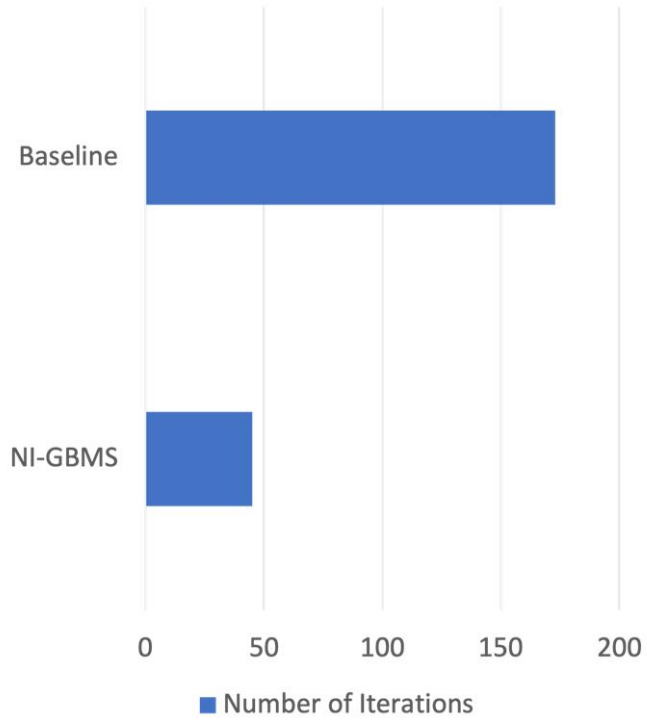


[2]S. Arisaka and Q. Li (2024) Accelerating Legacy Numerical Solvers by Non-intrusive Gradient-based Meta-solving

Preliminary result

We have applied the methodology to PETSc linear solver for Poisson equations by learning initial guesses and reduced the number of iterations by 74%.

We plan to apply it to learning turbulence models in OpenFOAM beyond linear solvers.



Future work

1. Generate a systematical dataset of the flow around bluffs; train SGS models within the dataset and design algorithms which improves the a-posteriori performance.

2. Deploy to practical problems: Subgrid-scale modeling in large eddy simulation of the urban environment.

3. Investigate the statistical and numerical properties of the data-driven turbulence modeling, with special focus on the dataset characteristic and the relation between data with different resolution.

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