Generative subgrid-scale modeling

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Summary

We study the data-driven subgrid-scale (SGS) modeling for the incompressible Navier-Stokes (NS) and the Kuramoto-Sivashinsky (KS) equations:

1. We explain the mismatch of "a-priori and a-posteriori dichotomy" by two features of the dataset: data imbalance and multi-valuedness.
2. We propose a generative modeling of the SGS stresses to resolve the multi-valuedness and demonstrate improvement in the simulation of the KS equation.

Dataset imbalance and multi-valuedness of SGS modeling

Applying a filter to the NS equations:

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j}, \quad \frac{\partial u_i}{\partial x_i} = 0,$$
$$\frac{\partial \widetilde{u}_i}{\partial t} + \widetilde{u}_j \frac{\partial \widetilde{u}_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \widetilde{p}}{\partial x_i} + \nu \frac{\partial^2 \widetilde{u}_i}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j}, \quad \frac{\partial \widetilde{u}_i}{\partial x_i} = 0,$$
$$\tau_{ij} = \widetilde{u_i u_j} - \widetilde{u}_i \widetilde{u}_j$$

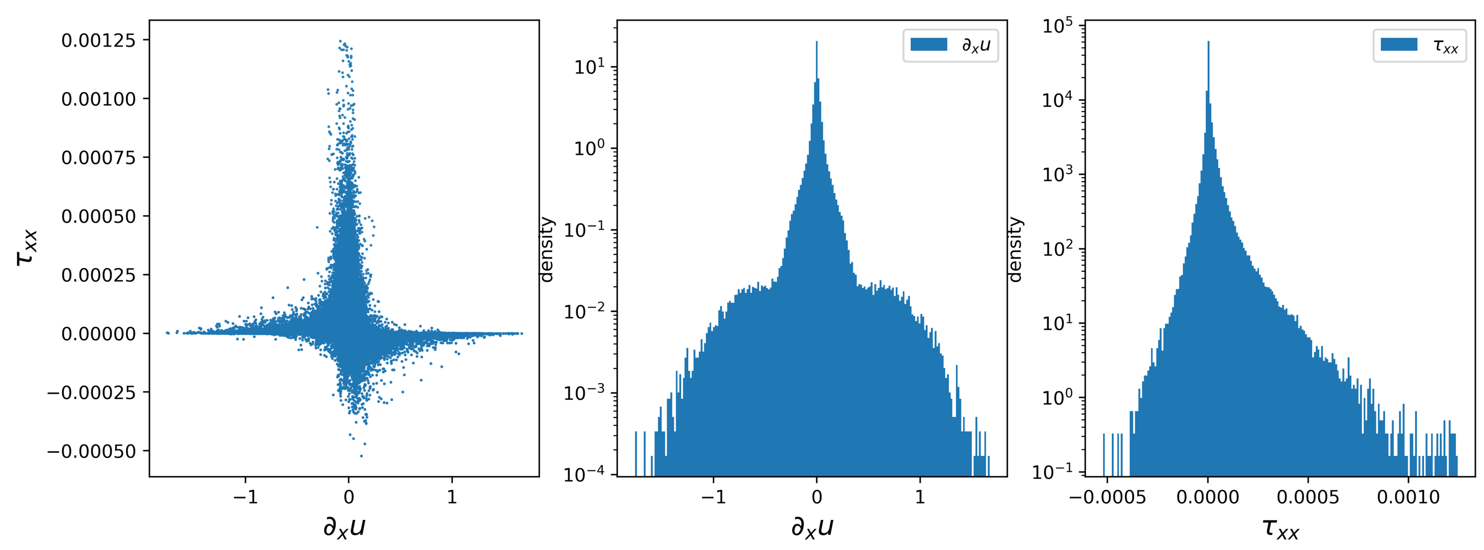
A closure term τ_{ij} appears because of the nonlinear convection.

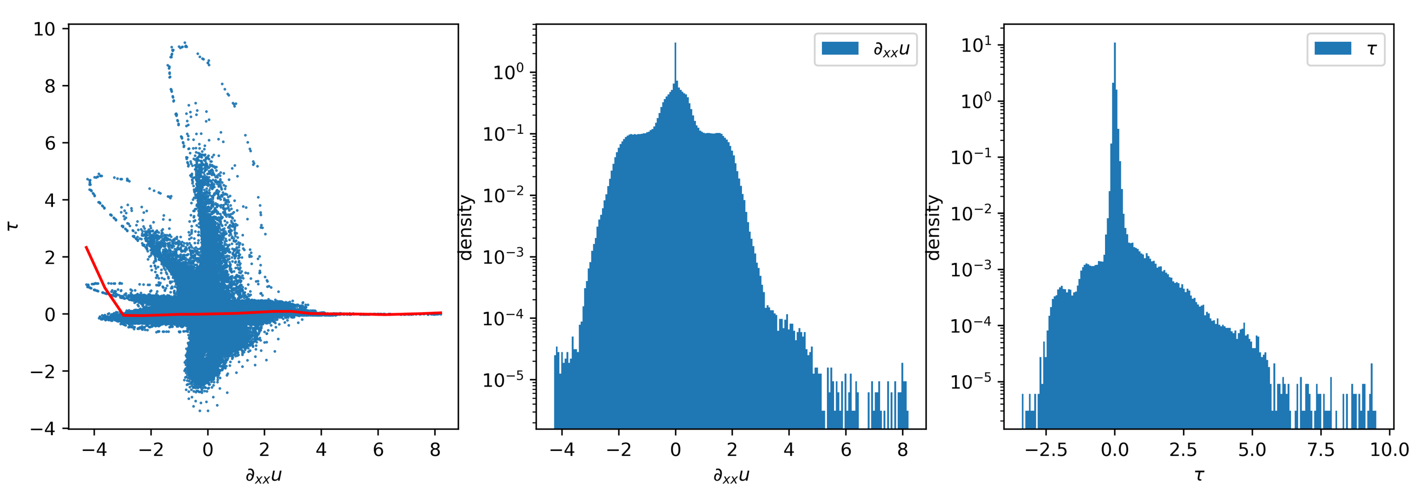
1. Classical modeling: empirical models, i.e. Smagorinsky model;
2. Data-driven SGS modeling: solve a regression problem:

$$\min_\theta \sum_n \left\| \phi_\theta(\widetilde{\mathbf{u}}^{(n)}) - \tau^{(n)} \right\|^2 .$$

Observations in literature:

1. **A large training error is inevitable.**
2. Data-driven models may **not improve the simulation accuracy** and even lead to blow up.





Our explanation:

1. **Data imbalance**: a large portion of data has negligible magnitude, causing the model hard to fit the dataset.
2. **Multivaluedness**: multiple values of stresses correspond to a single input, resulting in a large training error.

Proposed algorithm

To capture the multi-value nature of the SGS models, our solution is to **model the SGS stresses as a probability distribution conditioned on the input features**,

$$\tau = \phi_\theta(u) \quad \rightarrow \quad \tau \sim p_\theta(\cdot|u).$$

Using the Gaussian ansatz, one can optimize the likelihood function:

$$\max_\theta \sum_{i=n}^{N} \log p_\theta(\tau^{(n)}|u^{(n)}) \Longleftrightarrow \min_\theta \sum_{n=1}^{N} \frac{(\tau^{(n)} - \mu_\theta(u^{(n)}))^2}{2(\sigma_\theta(u^{(n)}))^2} + \log \sigma_\theta(u^{(n)}).$$

During the simulation, the new SGS stress term can be obtained via sampling:

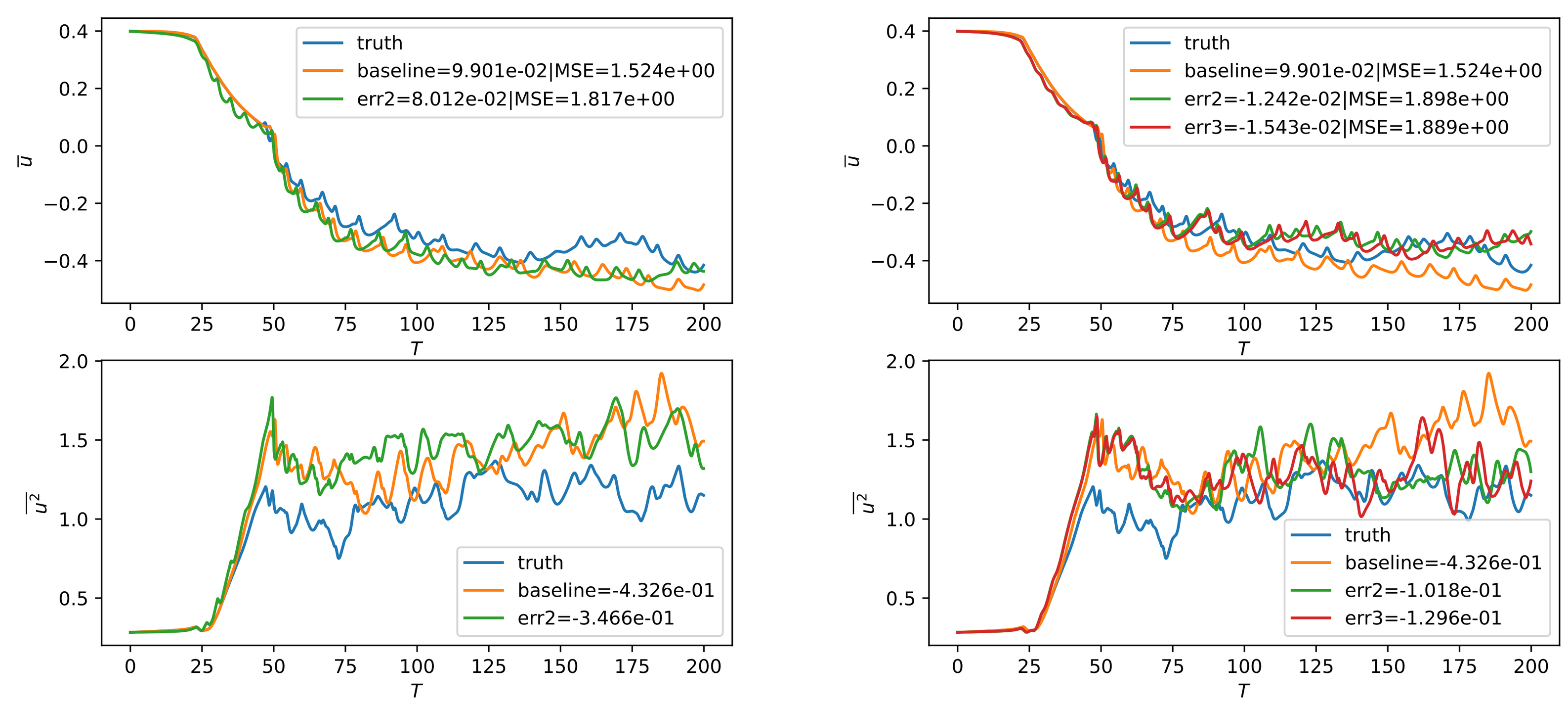
$$\tau(x,t) = \sigma_\theta(u(x,t))Z(x,t) + \mu_\theta(u(x,t)), \quad Z(t) \sim \mathcal{N}(0,1).$$

1. **Spatial consistency**: using the same Z for all x, i.e. $Z(x,t) = Z(t)$.
2. **Spatial-temporal consistency**: using the same Z for all x, t, i.e. $Z(x,t) = Z$.

Numerical experiments

We compare the following statistics to evaluate the a-posteriori performance.

$$\overline{u} = \frac{1}{LT}\int_0^L \int_0^T u(x,t)\,dt\,dx, \quad \overline{u^2} = \frac{1}{LT}\int_0^L \int_0^T u(x,t)^2\,dt\,dx,$$
$$\|u - u_0\|_2^2 = \frac{1}{LT}\int_0^L \int_0^T (u(x,t) - u_0(x,t))^2\,dt\,dx.$$



	baseline	regression	gaussian, fix	gaussian sample
a-priori error	N/A	0.976	-2.173	-2.173
$\int(u-u_0)^2 dxdt$	1.524	2.036	1.720	1.597
$\overline{u} - \overline{u_0}$	9.901E-02	1.011E-01	3.870E-02	3.214E-02
$\overline{u^2} - \overline{u_0^2}$	-4.326E-01	-4.241E-01	-1.895E-01	-6.577E-02
a-priori error	N/A	0.987	-2.583	-2.583
$\int(u-u_0)^2 dxdt$	1.524	1.817	1.898	1.889
$\overline{u} - \overline{u_0}$	9.901E-02	8.012E-02	-1.242E-02	-1.543E-02
$\overline{u^2} - \overline{u_0^2}$	-4.326E-01	-3.466E-01	-1.018E-01	-1.296E-01