
Normalizing Flows as a Novel PDF Turbulence Model

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Abstract

In this paper, we propose normalizing flows (NF) as a novel probability density function (PDF) turbulence model (NF-PDF model) for the Reynolds-averaged Navier-Stokes (RANS) equations. We propose to use normalizing flows in two different ways: firstly, as a direct model for the Reynolds stress tensor, and secondly as a second-moment closure model, i.e. for modeling the pressure-strain and dissipation tensor in the Reynolds stress transport equation. In classical PDF closure models, a stochastic differential equation has to be modeled and solved to obtain samples of turbulent quantities. The NF-PDF closure model allows for direct sampling from the underlying probability density functions of fluctuating turbulent quantities, such that ensemble-averaged quantities can then be computed. To illustrate this approach we demonstrate an application for the canonical case of homogeneous shear turbulence. Training data are extracted from high-fidelity direct numerical simulations (DNS).

1 Introduction

Turbulent flows are omnipresent in nature and engineering applications. Modeling and simulating turbulent flows have been a major challenge for decades. Complex spatio-temporal dynamics and strongly nonlinear behavior over multiple scales make direct numerical simulations of turbulent flows prohibitively expensive. Therefore, the development of reliable turbulence models with high predictive power is as important as ever before.

The Reynolds-averaged Navier-Stokes (RANS) equations are widely used in practical applications. Closure of the RANS equations is traditionally achieved by employing the turbulent viscosity hypothesis and isotropic closures, such as the prominent $k - \epsilon$ model. As such models generally fail to model anisotropy, the more fundamental Reynolds stress transport equations, so called second-moment closures, are used to provide higher fidelity [1]. Probability density function (PDF) methods provide an alternative modeling approach in which a transport equation for the one-point, one-time PDF of turbulent fluctuating quantities is solved [2, 3].

In recent years, with the emergence of machine learning, promising data-driven turbulence models have been developed [4]. Duraisamy and coworkers [5] have proposed deep learning enhancements of established RANS closure models, while Ling et al. [6] put forward a Galilean invariant neural network architecture for modeling the Reynolds stress anisotropy tensor. Beck et al. [7] used Deep Neural Networks for LES turbulence modelling, while Novati & Koumoutsakos [8] used reinforcement learning to adjust the Smagorinsky constant in LES simulations.

In this work, we propose a novel data-driven approach to RANS turbulence modelling which is in spirit close to the PDF modeling approach. We apply normalizing flows as a PDF-turbulence closure

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model (NF-PDF model). We examine the capabilities of normalizing flows to model the Reynolds stress tensor directly by learning the probability distribution of the fluctuating velocities as well as using normalizing flows for the closure of the Reynolds stress transport equation (RSTE). In the latter approach, the NF-PDF model learns the PDFs of the fluctuating pressure and the spatial gradient of the fluctuating velocities, thereby modeling the pressure-strain correlation and the dissipation term. We show proof of concept by the example of homogeneous shear turbulence (HST). Ground truth data are generated by direct numerical simulations. To the best of our knowledge, this work is the first time normalizing flows are used as PDF closure models.

In the next section we present the NF-PDF closure model. Section 3 presents the governing equations for HST. In section 4, we present results of the NF-PDF closure model for bounded and unbounded homogeneous shear turbulence. Finally, conclusions are given in section 5.

2 Normalizing Flows as a PDF Closure

Problem Statement

The Reynolds-averaged Navier-Stokes equations (1) contain the unclosed Reynolds stresses. In RANS turbulence modeling, often the Reynolds stresses $R_{ij} = \langle u'_i u'_j \rangle$ are modeled invoking an eddy viscosity hypothesis, e.g. with a two-equation model.

$$\frac{\partial \langle u_i \rangle}{\partial t} + \frac{\partial \langle u_i u_j \rangle}{\partial x_j} = - \frac{\partial \langle p \rangle}{\partial x_i} + \nu \frac{\partial^2 \langle u_i \rangle}{\partial x_j^2} - \frac{\partial \langle u'_i u'_j \rangle}{\partial x_j} \quad (1)$$

Here, u is the velocity, p is the pressure, and ν is the kinematic viscosity. $\langle \cdot \rangle$ represents an ensemble average, while $(\cdot)'$ is a fluctuating quantity. In Reynolds stress turbulence closure, transport equations for each component of the Reynolds stress tensor are solved. The unclosed terms in Eq. (2), i.e. pressure-strain $\Pi_{ij} = \langle p' \left(\frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i} \right) \rangle$ and dissipation $\epsilon_{ij} = 2\nu \langle \frac{\partial u'_i}{\partial x_k} \frac{\partial u'_j}{\partial x_k} \rangle$, have to be closed. P_{ij} is the turbulent production.

$$\frac{\partial R_{ij}}{\partial t} = P_{ij} + \Pi_{ij} - \epsilon_{ij} \quad (2)$$

Classical PDF methods model the transport equation for the one-point, one-time PDF of certain fluid properties, e.g. velocity [2, 9, 3]. Instead of solving the high-dimensional Fokker-Planck equation directly, Langevin methods are used. A set of particles is advected by a corresponding stochastic differential equation such that the particles have the same PDF as the underlying turbulent flow. Averaging over the particle ensembles yields estimates for the right-hand side of Eq. (2) in closed form given the sample means.

Normalizing Flows

In this work, we propose the normalizing flow PDF (NF-PDF) closure model for the RANS equations. The key idea of the NF-PDF model is to learn the underlying probability distributions of turbulent flow properties. Once the PDF is learned, straightforward sampling and successive ensemble-averaging from the NF model allows for very fast evaluation of the unclosed turbulent terms. Our approach circumvents the solution of stochastic differential equations (as in classical PDF methods) and can incorporate anisotropic flow conditions. The model also avoids adhoc closures that are part of state-of-the-art Reynolds stress models. A conditional NF-PDF model allows for time-dependent PDF, or PDF which are subject to given mean flow conditions. The NF-PDF model extends to high-dimensional problems enabling also to learn complex distributions over multiple variables, e.g. chemical compositions in turbulent reactive flows.

Normalizing flows are able to learn almost any probability distribution from data [10, 11, 12]. By applying a series of bijective transformations $g = f^{-1}$ to a simple prior probability distribution $p_Z(z)$, increasingly complex target distributions $p_X(x)$ can be approximated. Given the change of variable formula,

$$\log(p_X(\mathbf{x}|\mathbf{c}, \theta)) = \log(p_Z(f(\mathbf{x}|\mathbf{c}, \theta))) + \log \left| \det \left(\frac{\partial f(\mathbf{x}|\mathbf{c}, \theta)}{\partial \mathbf{x}^T} \right) \right|, \quad (3)$$

the model can be trained by minimizing the negative log-likelihood. In Eq. (3), θ are the trainable parameters of the flow, \mathbf{c} is a conditioning argument, and $\frac{\partial f(\mathbf{x}|\mathbf{c}, \theta)}{\partial \mathbf{x}^T}$ represents the Jacobian of f . At sampling time, a sample is drawn from the prior probability distribution p_Z . Applying the inverse transformation f^{-1} generates a sample in the original space $\mathbf{x} \sim p_X$.

Normalizing flows are often parameterized by neural networks which allow highly flexible transformations. In this work, we parameterize our normalizing flow with a sequence of real-valued non-volume preserving (real NVP) transformations [12]. RNVP makes use of affine coupling layers. The input to a RNVP layer $\mathbf{z} \in \mathbb{R}^D$ is split into two disjoint parts $(\mathbf{z}^A, \mathbf{z}^B) \in \mathbb{R}^d \times \mathbb{R}^{D-d}$. Then, the output of a single RNVP layer is calculated as

$$\mathbf{x}^A = \mathbf{z}^A \quad (4)$$

$$\mathbf{x}^B = \mathbf{z}^B \odot \exp(s(\mathbf{z}^A)) + t(\mathbf{z}^A), \quad (5)$$

where s and t are neural networks and \odot denotes element-wise multiplication. The Jacobian of said transformation is triangular which allows for efficient calculation of its determinant. We use an isotropic Gaussian as the prior $p_Z(\mathbf{z})$. A conditional version of the affine coupling layer was established in [13] which allows for conditional sample creation. The condition \mathbf{c} , e.g. mean flow conditions or time, is simply concatenated with the relevant input to the neural networks \mathbf{z}^A in Eq. (5).

3 Homogeneous Shear Turbulence (HST)

The reference dataset is generated from a 3D DNS of HST. HST is a canonical turbulent flow. The presence of a mean velocity gradient without disturbances from boundary effects makes HST the simplest non trivial turbulent shear flow. Experimental studies have been conducted by Corrsin and coworkers [14, 15]. Since Rogallo's pioneering work [16] many numerical investigations followed [17, 18, 19]. We employ Rogallo's method [16] and write the incompressible Navier-Stokes equations in a frame of reference moving with the mean shear flow $\langle u_1 \rangle = Sx_2$,

$$\frac{\partial u'_i}{\partial x_i^*} - St \frac{\partial u'_2}{\partial x_1^*} = 0, \quad (6)$$

$$\frac{\partial u'_i}{\partial t} + S\delta_{i1}u_2 + u'_j \frac{\partial u'_i}{\partial x_j^*} - St u'_2 \frac{\partial u'_i}{\partial x_1^*} = -\frac{\partial p'}{\partial x_i^*} + \nu \left(\frac{\partial^2 u'_i}{\partial (x_i^*)^2} + S^2 t^2 \frac{\partial^2 u'_i}{\partial (x_1^*)^2} - 2St \frac{\partial^2 u'_i}{\partial x_1^* \partial x_2^*} \right), \quad (7)$$

where u'_i is the fluctuating velocity, p' is the fluctuating pressure, and S is the shear rate. The comoving reference frame is related to the stationary reference frame by $x_i^* = x_i - St\delta_{i1}x_2$. Rogallo's transformation removes the explicit dependence of the Navier-Stokes equations on the spatial coordinate and allows the imposition of periodic boundary conditions. The equations are solved with an in-house parallelized pseudo-spectral code.

4 Results

4.1 Direct Reynolds Stress Tensor Modeling

The integral length scale in HST grows over time. Once it reaches the scale of the numerical domain, a statistically steady state can be reached in which turbulent energy production by mean shear and viscous energy dissipation are balanced. Fig. 1 shows the Reynolds stress components which become statistically stationary after an initial transient. Statistics are gathered once a statistically stationary state is reached.

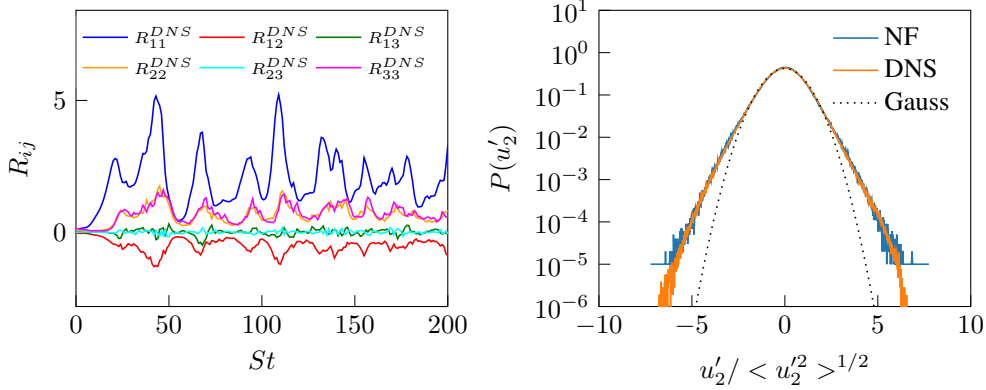


Figure 1: Left: Reynolds stress tensor over normalized time. Right: PDF of the u'_2 -velocity component with $n_{sample} = 10^7$. The dotted line is a Gaussian distribution with same mean and variance as the DNS data. Parameters of the HST flow are: $S = 1, \nu = 0.0015, Re = SL^2/\nu = 2632$.

Table 1: Components of the velocity anisotropy tensor b_{ij} .

Case	b_{11}	b_{22}	b_{33}	b_{12}
DNS	0.245	-0.128	-0.118	-0.159
NF, $n_{sample} = 10^3$	0.246	-0.126	-0.119	-0.166
NF, $n_{sample} = 10^5$	0.245	-0.125	-0.120	-0.160

We train an unconditional normalizing flow to learn the probability density distribution of the fluctuating velocities u'_i , i.e. $\mathbf{x} = \mathbf{u}' \in \mathbb{R}^3$. The fluctuating velocities show non Gaussian behavior in the x_2 and x_3 component, see for example Fig. 1 (right). Sampling from the NF model gives us u'_i , so that $R_{ij} = \langle u'_i u'_j \rangle$ can be easily computed. A RNVP flow of 8 coupling blocks is used. The neural networks in the affine coupling layers have three hidden layers with 64 neurons.

The NF accurately captures the PDF of the velocity components. By sampling from the NF and successive ensemble-averaging the Reynolds stress components can be calculated. Table 1 shows very accurate predictions for the Reynolds anisotropy tensor $b_{ij} = \langle u'_i u'_j \rangle / \langle u'_k u'_k \rangle - \delta_{ij}/3$ when compared to the DNS results.

4.1.1 Closure of the Reynolds Stress Transport Equation

In the initial transient state of HST, the Reynolds stresses are time dependent. We use a conditional NF to estimate the pressure-strain and dissipation tensor, which can then be used in the RSTE (2) to compute the Reynolds stresses. We learn the PDF of the velocity derivatives $p(\frac{\partial u'_i}{\partial x_j} | t)$ and of the fluctuating pressure $p(p' | t)$ conditioned on time t , i.e. $\mathbf{x} = (\frac{\partial u'_i}{\partial x_j}, p') \in \mathbb{R}^{10}$. An 8 layers RNVP flow is constructed with neural networks with three hidden layers each containing 128 hidden units. The time t is concatenated to \mathbf{x} and passed as an input to each RNVP layer.

The NF-PDF model accurately captures the dissipation term while the pressure-strain tensor prediction is adequate, see Fig. 2. In addition, the NF-PDF model yields very good predictive results when evaluated at time instances in between training points from the DNS. We observe a slight deviation from the DNS results in the Π_{11} component at early times. This error decreases with time.

5 Conclusion

We have presented a novel turbulence closure model on the basis of normalizing flows. In this proof of concept, we have shown that the NF-PDF closure model can successfully model the Reynolds stress tensor as well as the pressure-strain correlation and the dissipation tensor. As the pressure-strain

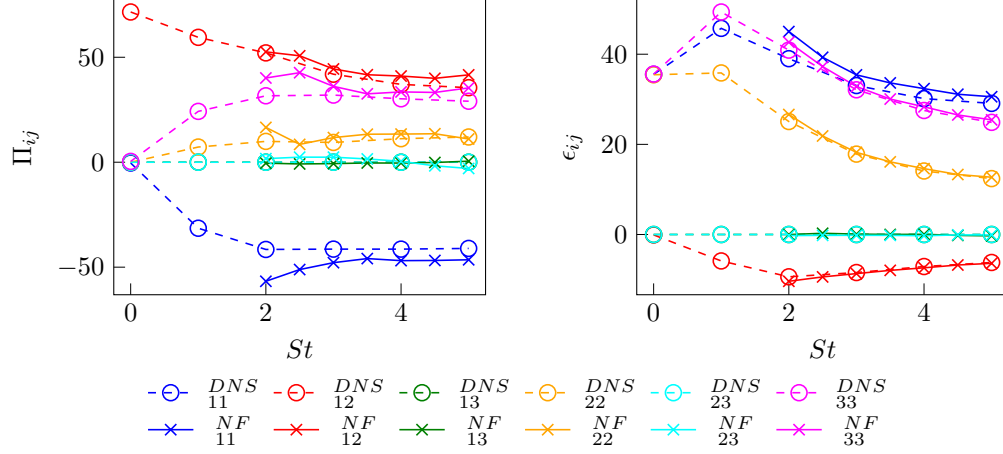


Figure 2: Pressure-strain correlation Π_{ij} (left) and dissipation ϵ_{ij} (right) over normalized time. The initialized velocity field is incompressible and isotropic. The NF-PDF model is fitted once a natural turbulent velocity field has developed ($St = 2$). $S = 20\sqrt{2}$, $\nu = 0.01/\sqrt{2}$, $Re = SL^2/\nu = 157914$.

tensor represents non-local interactions, its accurate prediction is particularly challenging. NF-PDF models have the potential to solve this key challenge of turbulence. Further research focuses on improving the prediction fidelity and on extending our method to more complex turbulent flows.

Broader Impact

Turbulent flows are omnipresent in nature and engineering applications. On the one hand, understanding turbulent flows plays an important role in the design of efficient engineering devices. For example, wind turbines rely heavily on the profound understanding of the incoming flow conditions, while turbulent mixing reduces emissions of combustion engines. On the other hand, the accurate simulation of turbulent atmospheric flows is crucial for weather forecasting. High-fidelity turbulence models play a central role in the prediction of hazardous weather events, e.g. hurricanes, air pollution, and wild fires. The authors recognize that their work contributes to both aforementioned aspects. Although the current work is still very much fundamental turbulence research, the authors are aware of its societal impact. At this point, the authors do not see any ethical concerns regarding the present work.

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