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Normalizing Flows as a Novel PDF Turbulence Model (NF-PDF Model)

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Turbulence modeling has been a major challenge for decades
Turbulent flows are omnipresent in nature and engineering applications. Turbulence modeling and simulation has been a major challenge for decades due to the nonlinear behavior and complex spatio-temporal dynamics.

Reynolds Averaged Navier Stokes equations need closure
In practical applications, the Reynolds averaged Navier Stokes (RANS) equations are widely used. RANS equations are transport equations for ensemble-averaged flow quantities, i.e. the averaged velocity and pressure field. The instantaneous velocity u_i can be decomposed into averaged part and fluctuating part as $u_i = < u_i > + u_i'$. RANS equations contain the unclosed Reynolds stresses $R_{ij} = < u_i' u_j' >$. The fluctuating velocities cannot be recovered from averaged quantities, R_{ij} has to be modeled.

$$\frac{\partial <u_i>}{\partial t} + \frac{\partial <u_i u_j>}{\partial x_i} = -\frac{\partial <p>}{\partial x_i} + \nu \frac{\partial^2 <u_i>}{\partial x_j^2} - \frac{\partial <u_i' u_j'>}{\partial x_j}$$

The closure problem can be deferred to a deeper level. In Reynolds stress turbulence closure, exact transport equations for the Reynolds stresses can be derived. However, the Reynolds stress transport equations (RSTE) themselves contain unclosed terms which need modelling, i.e. the pressure-strain correlation $\Pi_{ij} = < p' \left(\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i} \right) >$ and the dissipation $\epsilon_{ij} = 2\nu < \frac{\partial u_i'}{\partial x_k} \frac{\partial u_j'}{\partial x_k} >$.

$$\frac{\partial R_{ij}}{\partial t} = P_{ij} + \Pi_{ij} - \epsilon_{ij}$$

The fluctuating component of a turbulent quantity is a random variable.
The fluctuating component of a physical quantity in turbulent flows can be interpreted as a stochastic variable with a distinct underlying probability distribution [1]. In fact, PDF turbulence models solve an approximate Fokker-Planck for the PDF of the turbulent quantity.

The key idea of our NF-PDF ansatz is to learn the underlying probability density functions of the turbulent quantities from data. Once the PDFs are learned, we can sample from them, and subsequently calculate ensemble-averaged quantities explicitly. I.e., our procedure consist of the following three steps:

1. Learn the PDF of the fluctuating quantity $u' \sim p_{U'}(u')$
2. Draw N samples from the learned PDF $\{u_0', u_1', \ldots, u_N'\}$
3. Calculate averages over sampled set, e.g. $< u'u' > = \frac{1}{N} \sum u_i' u_i'$

Note, the training (step 1) has to be done only once before applying the NF-PDF model in a downstream task, i.e. RANS simulations.

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Normalizing Flows (NF)
Normalizing flows are able to learn almost any PDF $p_X(x)$ by applying a series of bijective transformations $g_\theta = f_\theta^{-1}$ to a simple prior probability distribution $p_Z(z)$, for example a Gaussian. Given the change of variable formula, the trainable parameters θ of the normalizing flow, often weights of a neural network, can be optimized by minimizing the negative log-likelihood

$$\log\big(p_X(x|c,\theta)\big) = \log\big(p_Z\big(f(x|c,\theta)\big)\big) + \log|\det(\frac{\partial f(x|c,\theta)}{\partial x})|$$

The PDF can have additional physical conditioning arguments c, e.g. mean flow conditions or time. $\partial f(x)/\partial x$ denotes the Jacobian of the transformation. In this work, we use real-valued non-volume preserving (RNVP) transformations [2]. The prior variable $z \in \mathbb{R}^D$ is split into two disjoint parts $(z^A, z^B) \in \mathbb{R}^{D-d} \times \mathbb{R}^d$. Then the transformation is applied as

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

where s and t are neural networks with trainable parameters θ.

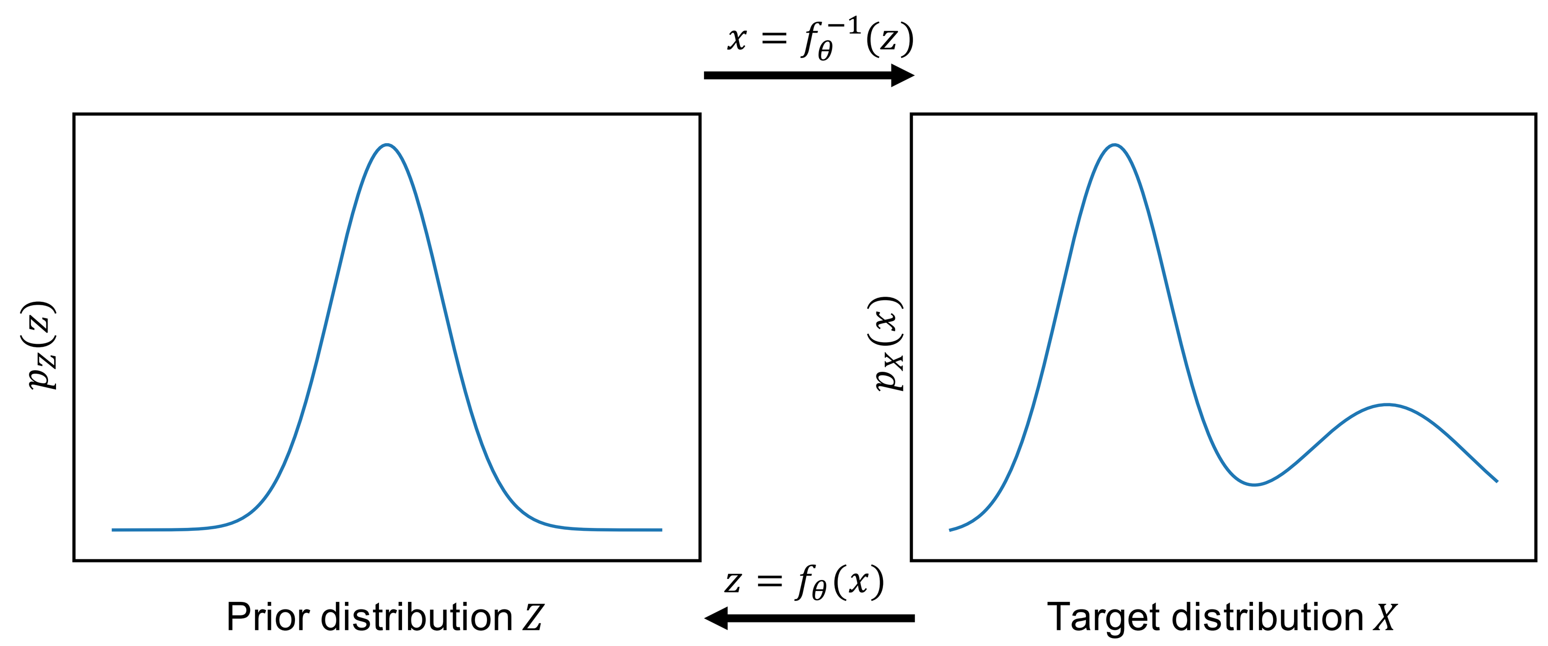

Figure 1. Change of variables. The bijective function f_θ^{-1} transforms the prior distribution to the target distribution.

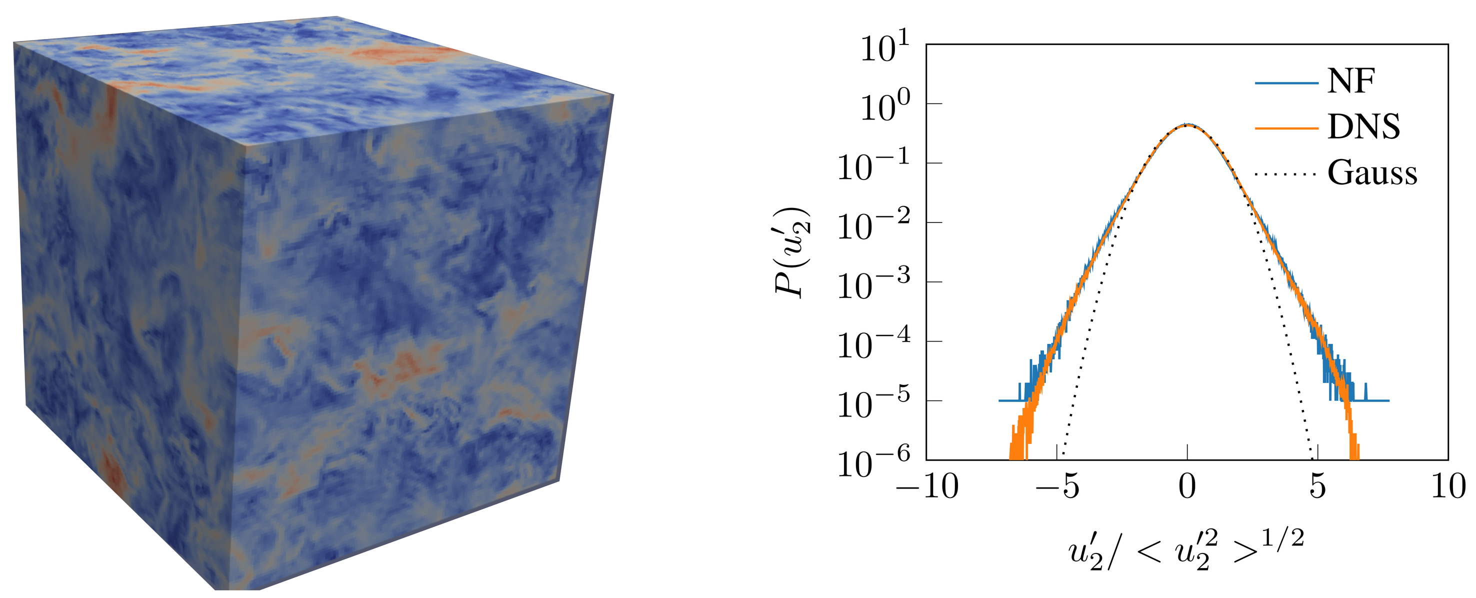

Figure 2. Left: Snapshot of a turbulent velocity field from HST. Right: PDF of the u_2' velocity showing non-Gaussian behavior.

Results for Homogeneous Shear Turbulence
We present results of the NF-PDF model for Homogeneous Shear Turbulence (HST). HST is a canonical turbulent shear flow. High fidelity data is obtained from Direct Numerical Simulations with a parallelized pseudo-spectral code.

We train an 8 layers RNVP with neural networks with three hidden layers with 64 neurons each to learn the PDF of the velocity fluctuations in a steady-state bounded HST. Figure 2 shows an instantaneous velocity field and the probability density function of the u_2'-component. The NF captures the PDF very accurately.

Before the HST reaches a steady-state, the Reynolds stresses are time-dependent in an initial transient phase. We use a conditional NF to learn $p(p'|t)$ and $p(\partial u_i'/\partial x_j|t)$ from which we can close the dissipation and pressure-strain correlation in the RSTE. Figure 3 shows that the NF-PDF model yields good predictive results, even when evaluated at time instances in between training points from the DNS.

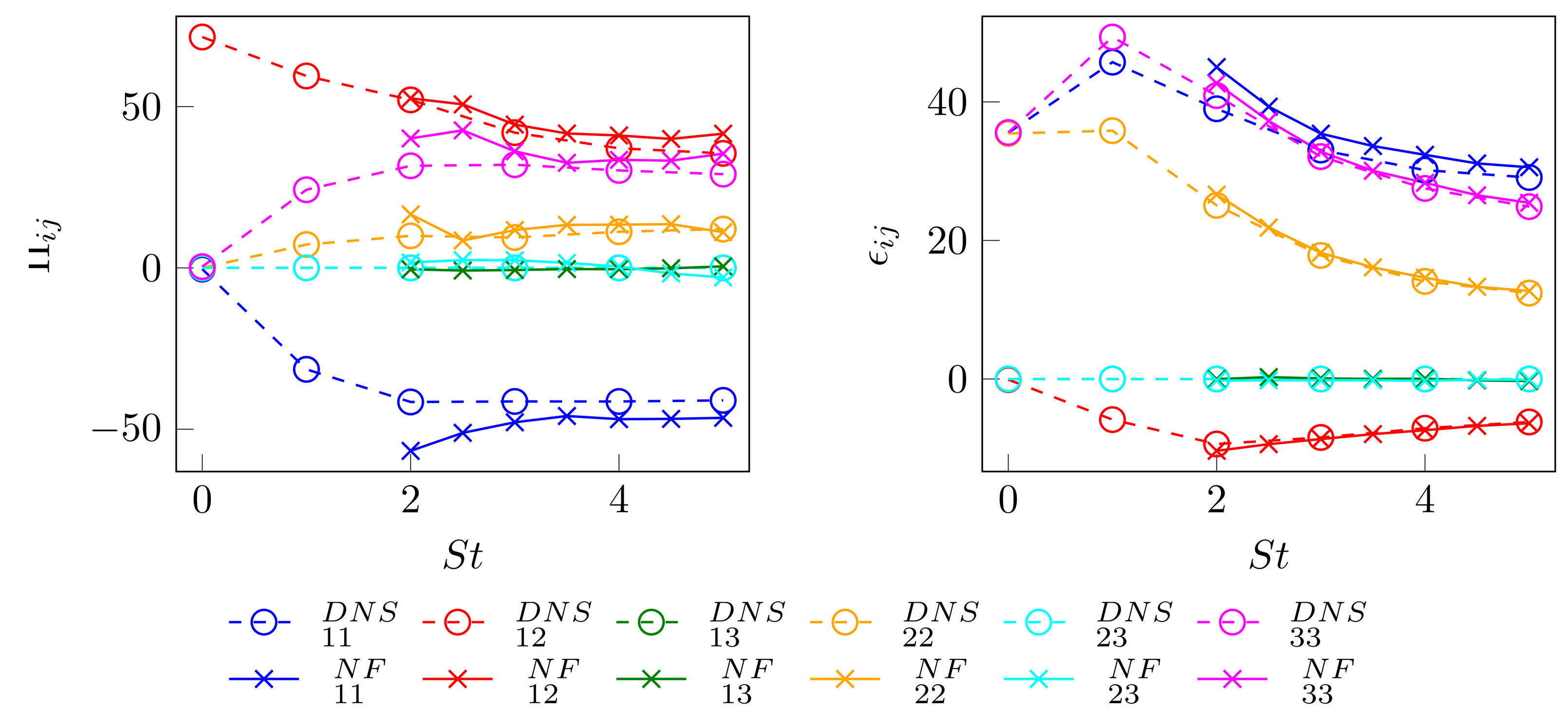

Figure 3. Pressure-strain correlation (left) and dissipation (right) over normalized time.

Conclusion
We have presented Normalizing Flow PDF turbulence models as a promising novel approach for successfully modelling the Reynolds stress tensor as well as the pressure-strain correlation and the dissipation tensor. NF-PDF models have the potential to close the RANS equations without adhoc closures. Further research focuses on increasing the predictive capabilities and on an extension to more complex turbulent flows.

References
[1] Stephen B Pope. *Turbulent flows.* Cambridge University Press, 2000.

[2] Laurent Dinh, Jascha Sohl-Dickstein, and Samy Bengio. *Density estimation using Real NVP.* arXiv preprint arXiv:1605.08803, 2016.