Using LES/DNS Data for Neural Network-based Improvement of Existing Turbulence Models

Mr. Jacob Welsh
Prof. Paul D. Orkwis

University of Cincinnati

Department of Aerospace Engineering and Engineering Mechanics

SOCHE
Strategic Ohio Council for Higher Education

NASA 2022 Symposium on Turbulence Modeling: Roadblocks and the Potential for Machine Learning

Turbulence Modeling Approaches

Traditional TM

Model the Reynolds stress (R_{ij})

- Boussinesq assumption, $R_{ij} \propto$ velocity gradients
- Utilize turbulence physics to improve

Examples

- Baldwin-Lomax 0-eq
- Spallart-Allmaras 1-eq
  - Transport eq. for isotropic ν_T
  - As many as 12 coefficients depending on PoV
  - Originally tuned to Samuel-Joubert flow and RAE 2822 airfoil
  - Many variations/improvements
- 2-eq/Algebraic R_{ij} models many more coefficients and variations

ML Enhanced TM

ML Assessment of Turbulence Physics

- Compute R_{ij} and turbulence source terms from LES/DNS data
- Determine how well existing turbulence models correlate to "truth" data
  - Directly assess the Boussinesq assumption
  - Directly assess derived turbulence physics

ML Optimization of TM model coefficients

- Experimental Objective Functions – Yoder and Orkwis
- Utilize LES/DNS "truth" data
- Local or global variable driven

ML Classification of Flows

- Ling and Templeton/Fuchi et al. variables

ML TM Development

- ML unsupervised learning to "discover" correlations between classification variables and equations based on them from LES/DNS data to derive new turbulence model forms

Reynolds Stresses

Back

- "Reynolds stress," R_{ij} ,is a consequence of the so-called Reynolds averaging process applied to the Navier-Stokes equations.

$$R_{ij} = -\rho\overline{u_i'u_j'}$$

- Derivatives of these terms appear in the Reynolds averaged Navier-Stokes equations (RANS).

$$\rho\bar{u}_j\frac{\partial \bar{u}_i}{\partial x_j} = \rho\bar{f}_i + \frac{\partial}{\partial x_j}\left[-\bar{p}\delta_{ij} + \mu\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right) - \rho\overline{u_i'u_j'}\right]$$

$\mu_l + \mu_t$

TST

https://en.wikipedia.org/wiki/Reynolds-averaged_Navier%E2%80%93Stokes_equations

- Boussinesq proposed that

$$-\overline{v_i'v_j'} = \nu_t\left(\frac{\partial \overline{v_i}}{\partial x_j} + \frac{\partial \overline{v_j}}{\partial x_i}\right) - \frac{2}{3}k\delta_{ij}$$

Which can be written in shorthand as

$$-\overline{v_i'v_j'} = 2\nu_t S_{ij} - \frac{2}{3}k\delta_{ij}$$

where S_{ij} is the mean rate of strain tensor

ν_t is the turbulence eddy viscosity

$k = \frac{1}{2}\overline{v_i'v_i'}$ is the turbulence kinetic energy

and δ_{ij} is the Kronecker delta.

https://en.wikipedia.org/wiki/Turbulence_modeling

R_{ij} and subsequently ν_t or μ_t can be computed directly from LES/DNS data, embodying all the modeling assumptions made in the scheme.

Turbulence Modeling

Turbulence Model Process

$$\bar{U} \rightarrow F(\bar{U}) \rightarrow \mu_T | Re_\sigma \rightarrow TST \quad \Rightarrow \quad \bar{U}_{Final}$$

Turbulence Model Optimization

$$F(\bar{U}_{Final}; c_1, \cdots, c_n)$$

$\bar{U}_{Final}$

$C_p, C_f, etc.$

Experimental Data

Objective Function

Requires 1 CFD solution for each set of coefficients

Algebraic Turbulence Models

- Johnson and King, Cebici and Smith, and Baldwin and Lomax invented models using Prandtl's mixing length idea to form algebraic turbulence models that work well near walls.

$$\mu_t = \begin{cases} \mu_{tinner} & \text{if } y \le y_{crossover} \\ \mu_{touter} & \text{if } y > y_{crossover} \end{cases}$$

Where $y_{crossover}$ is the smallest distance from the surface where μ_{tinner} is equal to μ_{touter}:

$$y_{crossover} = MIN(y) \ : \ \mu_{tinner} = \mu_{touter}$$

The inner region is given by the Prandtl - Van Driest formula:

$$\mu_{tinner} = \rho l^2 \left|\Omega\right|$$

$$\left|\Omega\right| = \sqrt{2\Omega_{ij}\Omega_{ij}}$$

$$\Omega_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i}\right)$$

The outer region is given by:

$$\mu_{touter} = \rho\, K\, C_{CP}\, F_{WAKE}\, F_{KLEB}(y)$$

Where

$$F_{WAKE} = MIN\left(y_{MAX}\, F_{MAX}\ ;\ C_{WK}\, y_{MAX}\, \frac{u_{DIF}^2}{F_{MAX}}\right)$$

y_{MAX} and F_{MAX} are determined from the maximum of the function:

$$F(y) = y\left|\Omega\right|\left(1 - e^{\frac{-y^+}{A^+}}\right)$$

F_{KLEB} is the intermittency factor given by:

$$F_{KLEB}(y) = \left[1 + 5.5\left(\frac{y\, C_{KLEB}}{y_{MAX}}\right)^6\right]^{-1}$$

u_{DIF} is the difference between maximum and minimum speed in the profile. For boundary layers the minimum is always set to zero.

$$u_{DIF} = MAX(\sqrt{u_i u_i}) - MIN(\sqrt{u_i u_i})$$

A^+	C_{CP}	C_{KLEB}	C_{WK}	k	K
26	1.6	0.3	0.25	0.4	0.0168

Introducing the essential idea of fitting coefficients to match experiments.

Notably:
Garabedian-Korn airfoil
Horstmann-Hung ramp
Hopkins-Inouye plate

https://www.cfd-online.com/Wiki/Baldwin-Lomax_model

Back

Spalart-Allmaras 1-eq Model

- Spalart and Allmaras created a 1-equation model for the transport of ν_t

$$\nu_t = \tilde{\nu} f_{v1}, \quad f_{v1} = \frac{\chi^3}{\chi^3 + C_{v1}^3}, \quad \chi := \frac{\tilde{\nu}}{\nu}$$

$$\frac{\partial \tilde{\nu}}{\partial t} + u_j \frac{\partial \tilde{\nu}}{\partial x_j} = C_{b1}[1 - f_{t2}]\tilde{S}\tilde{\nu} + \frac{1}{\sigma}\{\nabla \cdot [(\nu + \tilde{\nu})\nabla \tilde{\nu}] + C_{b2}|\nabla \tilde{\nu}|^2\} - \left[C_{w1} f_w - \frac{C_{b1}}{\kappa^2} f_{t2}\right] \left(\frac{\tilde{\nu}}{d}\right)^2 + f_{t1}\Delta U^2$$

$$\tilde{S} \equiv S + \frac{\tilde{\nu}}{\kappa^2 d^2} f_{v2}, \quad f_{v2} = 1 - \frac{\chi}{1 + \chi f_{v1}}$$

where

$$S = \equiv \sqrt{2\Omega_{ij}\Omega_{ij}}$$

$$\Omega_{ij} \equiv \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i}\right)$$

$$f_w = g \left[\frac{1 + C_{w3}^6}{g^6 + C_{w3}^6}\right]^{1/6}, \quad g = r + C_{w2}(r^6 - r), \quad r \equiv \frac{\tilde{\nu}}{\tilde{S}\kappa^2 d^2}$$

$$f_{t1} = C_{t1} g_t \exp\left(-C_{t2} \frac{\omega_t^2}{\Delta U^2}[d^2 + g_t^2 d_t^2]\right)$$

$$f_{t2} = C_{t3} \exp(-C_{t4}\chi^2)$$

d is the distance to the closest surface

The constants are

$$\begin{aligned}
\sigma &= 2/3 \\
C_{b1} &= 0.1355 \\
C_{b2} &= 0.622 \\
\kappa &= 0.41 \\
C_{w1} &= C_{b1}/\kappa^2 + (1 + C_{b2})/\sigma \\
C_{w2} &= 0.3 \\
C_{w3} &= 2 \\
C_{v1} &= 7.1 \\
C_{t1} &= 1 \\
C_{t2} &= 2 \\
C_{t3} &= 1.1 \\
C_{t4} &= 2
\end{aligned}$$

Up to 12 depending on how you count them. Their case was correlated against Samuel-Joubert and RAE 2822 airfoil

https://www.cfd-online.com/Wiki/Spalart-Allmaras_model

Back

Reynolds Stress Models

Which produce more and more coefficients.

Transport equations for R_{ij} are derived in Reynolds Stress Transport models

$$\frac{\partial}{\partial t}\left(-\tau^{T}_{ij}\right) + \frac{\partial}{\partial x_k}\left(-\tau^{T}_{ij}\tilde{u}_k\right) = \mathcal{P}_{ij} + \mathcal{D}_{ij} + \Pi_{ij} - \frac{2}{3}\bar{\rho}\epsilon\delta_{ij}$$

where the production, diffusion, and pressure-strain terms are

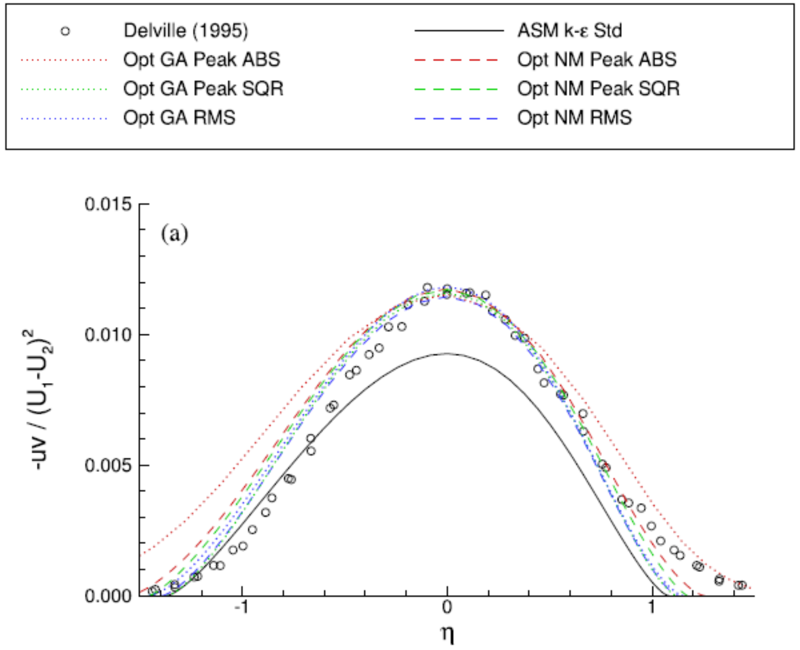
$$\mathcal{P}_{ij} = \tau^{T}_{ik}\frac{\partial \tilde{u}_j}{\partial x_k} + \tau^{T}_{jk}\frac{\partial \tilde{u}_i}{\partial x_k}$$

$$\mathcal{D}_{ij} = \frac{\partial}{\partial x_k}\left[\left(\mu_L + \frac{\mu_T}{\sigma_k}\right)\frac{\partial}{\partial x_k}\left(\frac{-\tau^{T}_{ij}}{\bar{\rho}}\right)\right]$$

$$\Pi_{ij} = -\left(C_1^0 + C_1^1\frac{\mathcal{P}}{\bar{\rho}\epsilon}\right)\bar{\rho}\epsilon b_{ij} + C_2\bar{\rho}k\tilde{S}^{D}_{ij} + C_3\bar{\rho}k\left[b_{ik}\tilde{S}_{kj} + \tilde{S}_{ik}b_{kj} - \frac{2}{3}b_{mn}\tilde{S}_{mn}\delta_{ij}\right] - C_4\bar{\rho}k\left[b_{ik}\tilde{R}_{kj} - \tilde{R}_{ik}b_{kj}\right]$$

An attempt at such modeling was made by Yoder and Orkwis using ML ideas against Delville's jet data.

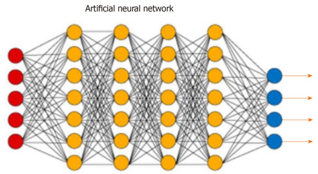
Yoder, D. A., & Orkwis, P. D. (2021). On the use of optimization techniques for turbulence model calibration. *Computers & Fluids*, *214*, 104752.



Back

ML Turbulence Modeling - 1

Turbulence Model Process



$$\bar{U} \rightarrow F(\bar{U}) \rightarrow \mu_T | Re_\sigma \rightarrow TST$$

$$\bar{U}_{Final}$$

Turbulence Model Optimization

$$F(\bar{U}_{Final}; c_1, \cdots, c_n)$$

$$\bar{U}_{Final}$$

$$C_p, C_f, etc.$$

Experimental Data

Objective Function

Requires 1 CFD solution for each set of coefficients

NN Model Accuracy

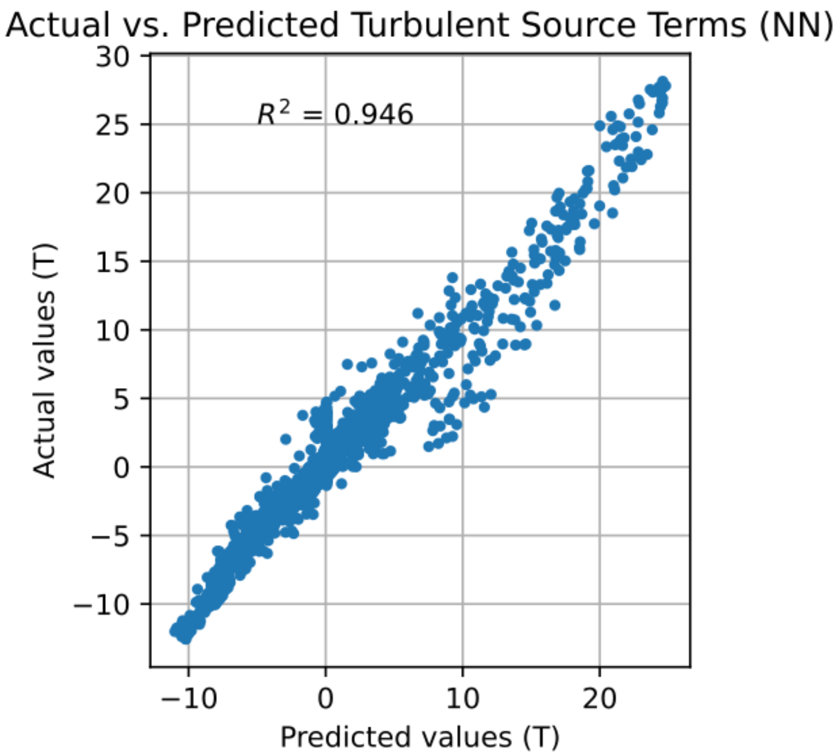
ML Model

TensorFlow NN used with a tanh loss function at all layers

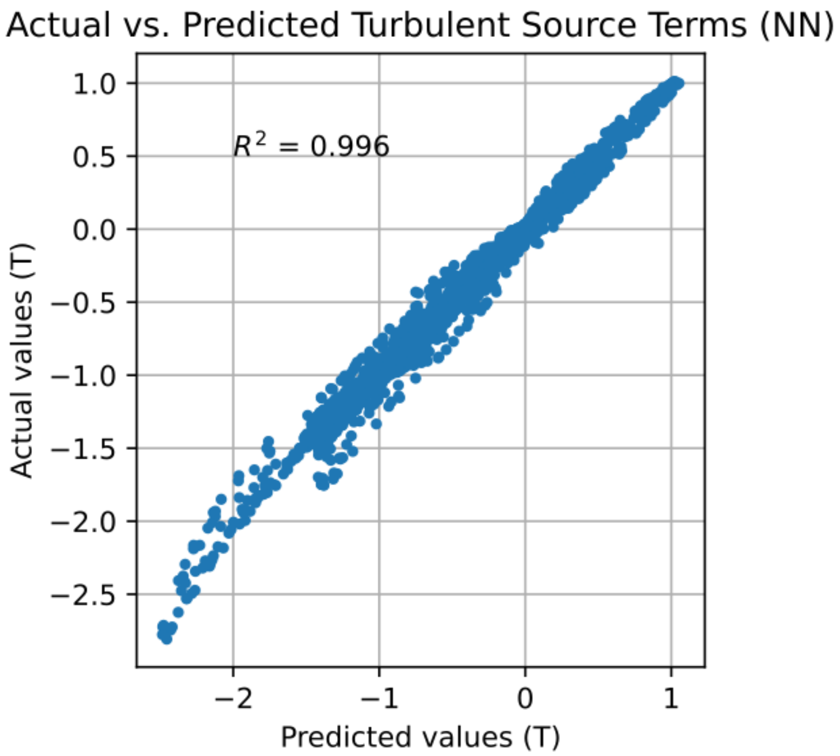
- **12 node input layer**
- **3 hidden layers of 30 nodes**
- **1 output**

To show validity of using a NN to fit lower fidelity data, used an 80-20 train-test split

Trained the X and Y turbulent source terms independently



X Turbulent Source Term



Y Turbulent Source Term

Turbulent Source Term

The inferred turbulent source term can be computed from the LES/DNS data. This is the term that should be compared to the turbulence model source term.

$$\rho \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} = \rho \bar{f}_i + \frac{\partial}{\partial x_j}\left[-\bar{p}\delta_{ij} + \mu\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right) - \rho \overline{u_i' u_j'}\right]$$

So that the governing equations become:

$$\rho \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} = \rho \bar{f}_i + \frac{\partial}{\partial x_j}\left[-\bar{p}\delta_{ij} + \mu\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right)\right] + \mathrm{T}_i$$

Where the LES/DNS data provides: $\mathrm{T}_i = -\frac{\partial \rho \overline{u_i' u_j'}}{\partial x_j}$

And turbulence modeling uses: $\widetilde{\mathrm{T}}_i = \frac{\partial}{\partial x_j}\left[\mu_t\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right)\right]$ or some variation.

ML Turbulence Modeling - 2

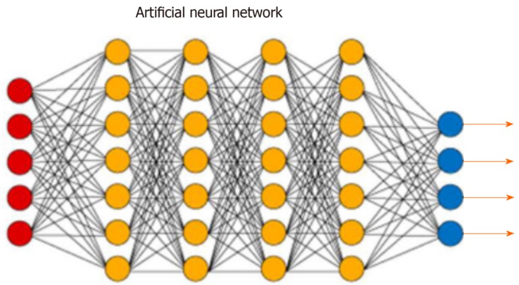
Turbulence Model Process

$$\bar{U} \rightarrow F(\bar{U}) \rightarrow \mu_T | Re_\sigma \rightarrow TST \quad \Rightarrow \quad \bar{U}_{Final}$$

Turbulence Model Optimization

$$F(\bar{U}(x,y,z); c_1, \cdots, c_n)$$

$$\bar{U}(x,y,z)$$



$$TST_{LES}(x,y,z)$$

$$TST(x,y,z)$$

Objective Function

Requires n CFD solutions – based on the n LES cases we want to employ

ML Turbulence Modeling - 3

Turbulence Model Process

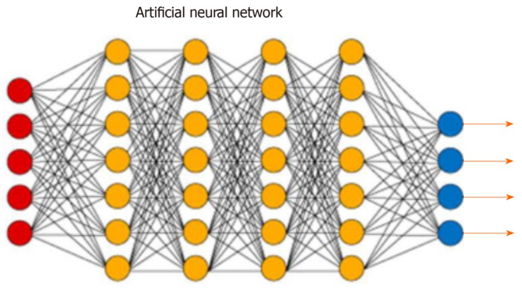
$$\bar{U} \rightarrow F(\bar{U}) \rightarrow \mu_T | Re_\sigma \rightarrow TST$$

$$\bar{U}_{Final}$$

Turbulence Model Optimization

$$F(\bar{U}(x,y,z); c_1(\bar{U}), \cdots, c_n(\bar{U}))$$

$$\bar{U}(x,y,z)$$



$$TST_{LES}(x,y,z)$$

$$TST(x,y,z)$$

Objective Function

Requires n CFD solutions – based on the n LES cases we want to employ

Classification: Ling and Templeton Variables

085103-11 J. Ling and J. Templeton Phys. Fluids **27**, 085103 (2015)

TABLE II. Non-dimensional inputs.

#	Description	Formula	#	Description	Formula
1	Non-dimensionalized Q criterion	$\frac{\|R\|^2-\|S\|^2}{\|R\|^2+\|S\|^2}$	7	Ratio of pressure normal stresses to normal shear stresses	$\frac{\sqrt{\frac{\partial P}{\partial x_i}\frac{\partial P}{\partial x_i}}}{\sqrt{\frac{\partial P}{\partial x_j}\frac{\partial P}{\partial x_j}}+0.5\rho\frac{\partial U_k^2}{\partial x_k}}$
2	Turbulence intensity	$\frac{k}{0.5U_iU_i+k}$	8	Vortex stretching	$\frac{\sqrt{\omega_j\frac{\partial U_i}{\partial x_j}\omega_k\frac{\partial U_i}{\partial x_k}}}{\sqrt{\omega_l\frac{\partial U_n}{\partial x_l}\omega_m\frac{\partial U_n}{\partial x_m}}+\|S\|}$
3	Turbulence Reynolds number	$\min(\frac{\sqrt{k}\,d}{50\nu},2)$	9	Marker of Gorle *et al.*,[13] deviation from parallel shear flow	$\frac{\lvert U_kU_l\frac{\partial U_k}{\partial x_l}\rvert}{\sqrt{U_nU_nU_i\frac{\partial U_i}{\partial x_j}U_m\frac{\partial U_m}{\partial x_j}}+\lvert U_iU_j\frac{\partial U_i}{\partial x_j}\rvert}$
4	Pressure gradient along streamline	$\frac{U_k\frac{\partial P}{\partial x_k}}{\sqrt{\frac{\partial P}{\partial x_j}\frac{\partial P}{\partial x_j}U_iU_i}+\lvert U_l\frac{\partial P}{\partial x_l}\rvert}$	10	Ratio of convection to production of k	$\frac{U_i\frac{dk}{dx_i}}{\lvert\overline{u'_ju'_l}S_{jl}\rvert+U_l\frac{dk}{dx_l}}$
5	Ratio of turbulent time scale to mean strain time scale	$\frac{\|S\|k}{\|S\|k+\epsilon}$	11	Ratio of total Reynolds stresses to normal Reynolds stresses	$\frac{\|\overline{u'_iu'_j}\|}{k+\|\overline{u'_iu'_j}\|}$
6	Viscosity ratio	$\frac{\nu_t}{100\nu+\nu_t}$	12	Cubic eddy viscosity comparison	$\frac{S_{ij}(\overline{u'_iu'_j}_{CEVM}-\overline{u'_iu'_j}_{LEVM})}{S_{kl}(\overline{u'_ku'_l}_{CEVM}+\overline{u'_ku'_l}_{LEVM})}$

Back

What’s Needed…

- Clean LES/DNS data that has been run sufficiently long for meaningful statistical data.
  - High quality grids
  - Sufficient T_c
  - Mean flow solution throughout the field
  - Reynolds stresses throughout the field
  - Able to create TSTs at each point
- A good idea of what variables best characterize a flow.
  - Including the scale at which to characterize (global, local, cell).
- A broad range of “different” solutions.

Acknowledgements

Thank you

- Dr. Chris Schrock
- Dr. Phil Beran
- Dr. Kazuko Fuchi
- Dr. Eric Wolf
- Air Force Summer Faculty/Graduate Student Fellowship Programs
- Dayton Area Graduate Studies Institute/Southeast Ohio Council for Higher Education

Questions?