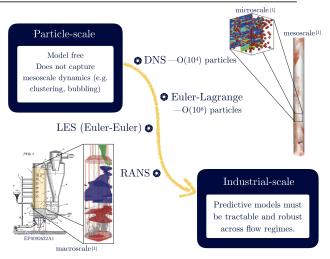
# Sparse identification of multiphase RANS closures

Sarah Beetham, Jesse Capecelatro University of Michigan, Ann Arbor



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# Challenges in multiphase turbulence modeling



[1] Tenneti and Subramaniam (2014)



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# Objectives and outline

**Objective:** Develop accurate and predictive multiphase turbulence models that capture relevant physics across scales.

#### Agenda:

- Canonical flow to isolate 2-way coupling in turbulence
  - ► Fully-developed cluster induced turbulence (CIT)
  - Numerical framework for generating data
  - Shortcomings of existing closure models
- The role of machine learning in turbulence modeling
- Sparse identification
  - ► Application to single-phase turbulence
  - Application to fully-developed CIT
- Looking ahead



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# Fully-developed, cluster-induced turbulence <sup>1</sup><sup>2</sup>

- Requires a mean velocity difference between phases (e.g. body forces (gravity), inlet conditions)
- Mass loading  $\varphi = \frac{\rho_p}{\rho_f} \frac{\langle \alpha_p \rangle}{\langle \alpha_f \rangle} \gtrsim 1$
- Spontaneous cluster formation
  - Characteristic timescale  $\tau_p = \frac{\rho_p}{\rho_f} \frac{d_p^2}{18\nu_f}$
  - Terminal velocity  $\mathcal{V} = \tau_p g$
  - Particle Reynolds number  $\operatorname{Re}_p = \frac{\mathcal{V}d_p}{\nu_{\epsilon}}$
  - Cluster size  $\mathcal{L} = \tau_p^2 g \gg d_p$
- Fluctuations in  $\alpha_p$  can generate and sustain fluid-phase turbulence (fully-developed CIT)
- In the absence of mean shear, turbulent kinetic energy is produced by two-way coupling through drag (Drag Production).

We consider the most simplified two-way coupled flow.

 J. Capecelatro et al. (2014), J. Fluid Mech., [2] Agrawal, Sundaresan, et al. (2001), J. Fluid Mech.



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# Eulerian-Lagrangian solution of mesoscale equations

- NGA<sup>3</sup>
  - Finite volume DNS/LES code
  - Conservation of mass, momentum and kinetic energy

Interphase momentum exchange

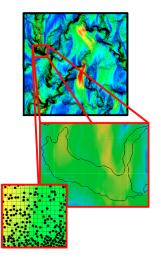
$$\frac{\partial \alpha_f \mathbf{u}_f}{\partial t} + \nabla \cdot \alpha_f \mathbf{u}_f \otimes \mathbf{u}_f = -\frac{1}{\rho_f} \nabla p_f + \frac{1}{\rho_f} \cdot \nabla \cdot \boldsymbol{\sigma}_f - \alpha_f \varphi \mathcal{A} + \alpha_f \mathbf{g}$$

- Lagrangian particle tracking<sup>4</sup>
  - Newton's 2nd law for particle position and velocity
  - 2nd-order Runge-Kutta for particle ODEs
  - Soft-sphere collision model
- Interphase exchange

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- Particle volume fraction and momentum transferred to fluid
- Fully conservative and consistent filtering approach<sup>4</sup>
- Transferred data converges under mesh refinement

[3] Desjardins et al. (2008) [4] Capecelatro et al. (2013)



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Sparse Identification

# Simulation results

1.00.30.10.001 0.01 0.1  $\langle \alpha_p \rangle$ 



 ${\rm Re}_p$ 

• Mesh: 512×512  $(896\,d_p \times 896\,d_p)$ 

- $\bullet N_p = (12,359 \ 57,362 \ 266,278)$
- $\bullet$  Enforce mass flow rate = 0

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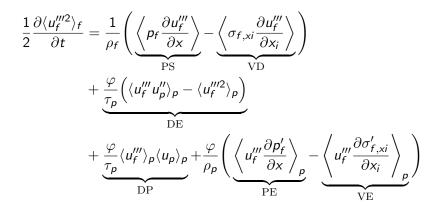
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Background Fully developed CIT Sparse Identification Looking ahead

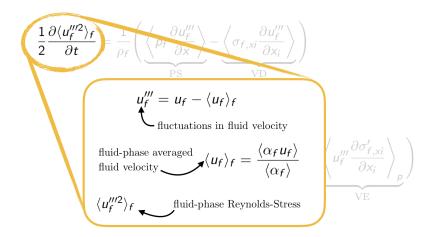
# RANS equations for fully-developed CIT

Phase-averaging of the mesoscale equations allow us to arrive at the RANS equations for fully-developed CIT.<sup>5</sup>  $^{6}$ 



[5] R. Fox (2014), JFM, [6] Capecelatro et al (2015), JFM

# RANS equations for fully-developed CIT





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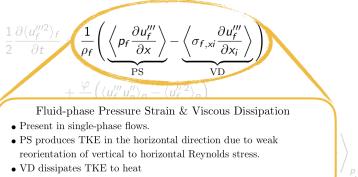
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Sparse Identification

Looking ahead

# RANS equations for fully-developed CIT



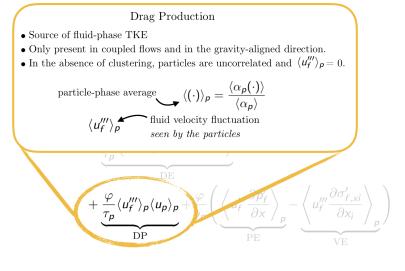
•  $\sigma_{f,xi}$  is the viscous stress tensor.



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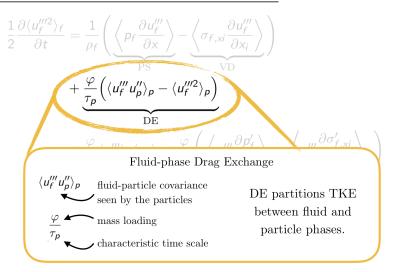
# RANS equations for fully-developed CIT





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# RANS equations for fully-developed CIT





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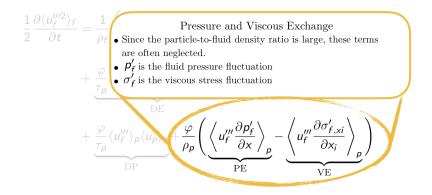
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Background Fully developed CIT Sparse Identification

Looking ahead

# RANS equations for fully-developed CIT





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Unclosed terms are typically modeled by extension from single-phase  $\mathrm{flow}^4$ 

Pressure Strain & Viscous Dissipation:

$$\frac{1}{\rho_f} \left( \left\langle p_f \frac{\partial u_f'''}{\partial x} \right\rangle - \left\langle \sigma_{f,xi} \frac{\partial u_f'''}{\partial x_i} \right\rangle \right) = -C_{Rf} \frac{\varepsilon_f}{k_f} \left( \langle u_f'''^2 \rangle_f - k_f \right) - \varepsilon_f$$

Drag Exchange:

$$\frac{\varphi}{\tau_p} \Big( \langle u_f^{\prime\prime\prime} u_p^{\prime\prime} \rangle_p - \langle u_f^{\prime\prime\prime2} \rangle_p \Big) = \frac{\varphi}{\tau_p} \left( \beta_{fp,1} \langle u_f^{\prime\prime\prime2} \rangle_f^{1/2} \langle u_p^{\prime\prime2} \rangle_p^{1/2} - \beta_{f,1} \langle u_f^{\prime\prime\prime2} \rangle_f \right)$$

Drag Production:

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$$\begin{split} \frac{\varphi}{\tau_p} \langle u_f^{\prime\prime\prime} \rangle_p \langle u_p \rangle_p &= \frac{\varphi}{\tau_p} C_g \langle u_p \rangle_p^2 \\ \text{where } C_g &= \frac{\langle u_f^{\prime\prime\prime} \rangle_p}{\langle u_p \rangle_p} \end{split}$$

Pressure and Viscous Exchange Terms are assumed to be negligible.

[4] Fox, R. (2014); Capecelatro *et al.* (2015)

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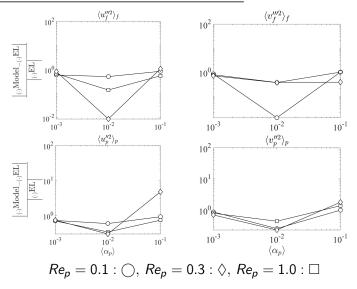
$$\frac{\varphi}{\tau_p} \Big( \langle u_f^{\prime\prime\prime} u_p^{\prime\prime} \rangle_p - \langle u_f^{\prime\prime\prime2} \rangle_p \Big) = \frac{\varphi}{\tau_p} \left( \beta_{fp,1} \langle u_f^{\prime\prime\prime2} \rangle_f^{1/2} \langle u_p^{\prime\prime2} \rangle_p^{1/2} - \beta_{f,1} \langle u_f^{\prime\prime\prime2} \rangle_f \right)$$

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Pressure and Viscous Exchange Terms are assumed to be negligible.

# Existing closures fail to be predictive





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Closures adapted from single-phase break down for even the most simplified two-way coupled flows

# Can machine learning provide a tractable closure?



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Background Fully developed CIT

Sparse Identification

Looking ahead

# Machine learning in CFD

Neural Networks<sup>5</sup> and Sparse Regression<sup>6</sup> are key players in data-driven turbulence modeling.

Neural Networks

#### Benefits

- Complete generality
- Requires no prior knowledge of underlying physics

Drawbacks

• Difficult to express in compact form

Sparse Regression

# Benefits

- Compact, algebraic form
- Model selection *and* regression
- Easily incorporated into CFD solvers

#### Drawbacks

• Relies on modeler to select appropriate test functions

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[5] Duraysami et al (2018) [6] Brunton et al (2016)

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Sparse Identification

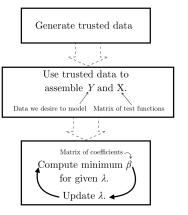
# Sparse identification

We define the sparse model as

$$\mathbf{y} = \mathbf{X}\hat{\beta}.$$

Determining the optimal coefficient matrix is cast as a sparse minimization problem

$$\hat{\beta} = \min_{\beta} \underbrace{||y - X\beta||_2^2}_{\text{regression}} + \underbrace{\lambda||\beta||_1}_{\text{sparcity}}$$



Demonstrated success for classical, dynamic systems (e.g. the Lorenz attractor).<sup>6</sup> Can this technique be applied successfully to realistic flows?

[6] Brunton et al (2016)



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# Sparse identification

Agenda:

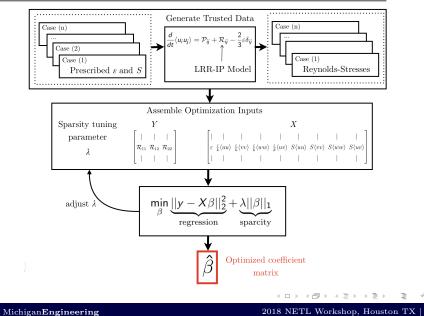
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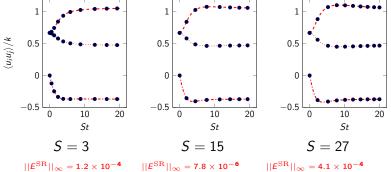
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# Sparse Regression method applied to synthetic data



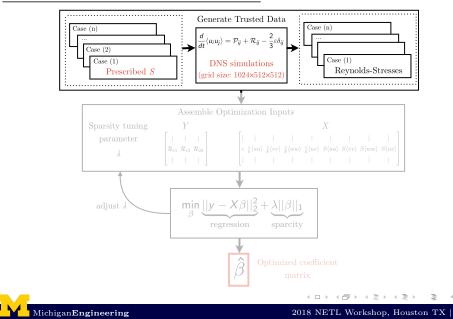
#### Sparse identification correctly returns the LRR-IP model

Equation	ε	$\frac{\varepsilon}{k}\langle uu\rangle$	$\frac{\varepsilon}{k} \langle uv \rangle$	$\frac{\varepsilon}{k}\langle vv \rangle$	$\langle uu \rangle \frac{\partial \langle u \rangle}{\partial y}$	$\langle vv \rangle \frac{\partial \langle u \rangle}{\partial y}$	$\langle uv \rangle \frac{\partial \langle u \rangle}{\partial y}$
$\mathcal{R}_{1,1}$	$\frac{2}{3}C_R$	$-C_R$	0	0	0	0	$\frac{4}{3}C_{2}$
$\mathcal{R}^{\mathrm{SIMR}}_{1,1}$	1.2056	-1.8054	0	0	0	0	0.79999
$\mathcal{R}_{1,2}$	0	0	$-C_R$	0	0	C2	0
$\mathcal{R}_{1,2}^{\mathrm{SIMR}}$	0	0	-1.79956	0	0	0.600055	0
$\mathcal{R}_{2,2}$	$\frac{2}{3}C_R$	0	0	$-C_R$	0	0	$-\frac{2}{3}C_2$
$\mathcal{R}^{\mathrm{SIMR}}_{2,2}$	1.197513	0	0	-1.79956	0	0	-0.40038





# DNS-generated shear turbulence



Background Fully developed CIT Sparse Identification

Looking ahead

# DNS-generated homogeneous shear turbulence

Equation	ε	$\frac{\varepsilon}{L} \langle uu \rangle$	$\frac{\varepsilon}{L} \langle vv \rangle$	$\frac{\varepsilon}{L} \langle ww \rangle$	$\frac{\varepsilon}{L} \langle uv \rangle$	S (uu)	S(vv)	S(ww)	S(uv)
$\mathcal{R}_{1,1}^{\mathrm{LRR-IP}}$	$\frac{2}{3}C_R$	$-C_R$	0	0	0	0	0	0	$-\frac{4}{3}C_{2}$
$\mathcal{R}_{1,1}^{\mathrm{SIMR}}$	43.32	-20.07	0	-48.98	-20.36	0	-1.95	2.03	3.04
RLRR-IP	0	0	$-C_R$	0	0	-C2	0		
$\mathcal{R}_{1,2}^{\mathrm{SIMR}}$	10.38	-6.37	0	-2.70	8.74	0	0.65	0	-0.45
$\mathcal{R}_{2,2}^{\mathrm{LRR-IP}}$	$\frac{2}{3}C_R$	0	0	$-C_R$	0	0	$\frac{2}{3}C_{2}$		
$\mathcal{R}_{2,2}^{SIMR}$	-5.09	3.38	0	-4.99	-17.51	0	0.42	0	0.41
$\mathcal{R}_{3.3}^{\mathrm{LRR-IP}}$	$\frac{2}{3}C_R$	0	0	$-C_R$	0	0	$\frac{2}{3}C_{2}$		
$\mathcal{R}_{3,3}^{\mathrm{SIMR}}$	-11.17	8.12	0	-4.14	-21.29	0	0.81	0	0.99

#### Discovered sparse identification model

# LLR-IP model<sup>7</sup> $\mathcal{R}_{ij} = -C_R \frac{\varepsilon}{\iota} \left( \langle u_i u_j \rangle - \frac{2}{3} k \delta_{ij} \right) - C_2 \left( \mathcal{P}_{ij} - \frac{2}{3} \mathcal{P} \delta_{ij} \right)$

with typical values  $C_R = 1.8$  and  $C_2 = 3/5$ .

Model identified by sparse identification  $\begin{aligned} &\mathcal{R}_{1,1} = 28\frac{\varepsilon}{k}\left(\langle uu\rangle + 5/3\langle vv\rangle - 0.7\langle uv\rangle - 1.9k\right) - 2S\langle vv\rangle + 2S\langle ww\rangle + 3S\langle uv\rangle \\ &\mathcal{R}_{1,2} = 2.7\frac{\varepsilon}{k}\left(-1.4\langle uu\rangle + \langle vv\rangle + 3.2\langle uv\rangle + 1.9k\right) + 0.6S\langle vv\rangle - 0.4S\langle uv\rangle \\ &\mathcal{R}_{2,2} = 5\frac{\varepsilon}{k}\left(1.67\langle uu\rangle + \langle vv\rangle - 3.5\langle uv\rangle - 3k\right) - 0.4S\langle vv\rangle + 0.4S\langle uv\rangle \\ &\mathcal{R}_{3,3} = 4\frac{\varepsilon}{k}\left(3\langle uu\rangle + \langle vv\rangle - 5\langle uv\rangle - 4.7k\right) - 0.8S\langle vv\rangle + S\langle uv\rangle \end{aligned}$ 

[7] Pope, S. (2012) Cambridge Univ. Press

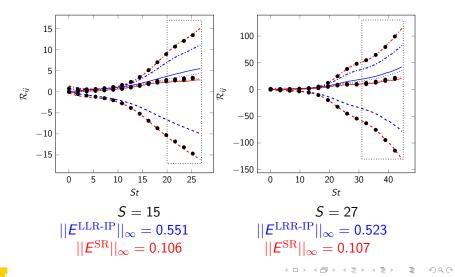
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DNS-generated homogeneous shear turbulence

Sparse identification model out performs LRR-IP model

Background Fully developed CIT Sparse Identification Looking ahead





# Sparse identification

Agenda:

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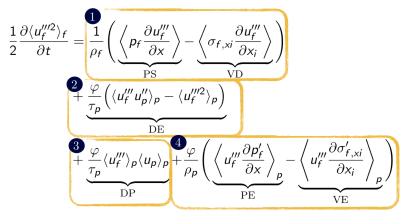
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Background Fully developed CIT Sparse Identification

Looking ahead

# Sparse identification of fully-developed CIT

We group the unclosed terms and conduct sparse identification for the four terms using highly-resolved data generated using NGA.





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# Sparse identification of fully-developed CIT

$$\frac{1}{\rho_{f}} \left( \underbrace{\left\langle p_{f} \frac{\partial u_{f}''}{\partial x} \right\rangle}_{\text{PS}} - \underbrace{\left\langle \sigma_{f,xi} \frac{\partial u_{f}''}{\partial x_{i}} \right\rangle}_{\text{VD}} \right) = C_{Rf} \frac{\varepsilon_{f}}{k_{f}} \left( \langle u_{f}''^{2} \rangle_{f} - k_{f} \right) - \varepsilon_{f}$$
Exact expression Existing Closure
$$Closure \text{ Discovered by Sparse Regression} = -1.1 \frac{\varepsilon_{f}}{k_{f}} \langle u_{f}''^{2} \rangle + \frac{\varphi}{\tau_{p}} \left( 0.004 \langle v_{f}''^{2} \rangle + (0.02Re_{p} + 0.14 \langle \alpha_{p} \rangle - 0.02) \langle u_{f}''^{2} \rangle \right) \\
+ \frac{\varphi}{\tau_{p}} \left( \left( 0.06Re_{p} + 0.05 \right) \langle u_{p}''^{2} \rangle_{p} - 0.13 \langle v_{p}''^{2} \rangle_{p} \right) - 0.13Re_{p} \frac{\varphi}{\tau_{p}} \langle u_{f}'''^{2} \rangle^{\frac{1}{2}} \langle u_{p}''^{2} \rangle_{p}^{\frac{1}{2}}$$

Existing Model Error

		0.001	$\langle \alpha_p \rangle$ 0.01	0.1
	0.1	0.66	0.83	0.89
Rep	0.3	0.53	0.92	0.97
1	1.0	0.77	0.92	0.98

Sparse identification Error

			$\langle \alpha_p \rangle$	
		0.001	0.01	0.1
	0.1	$0.7 \times 10^{-14}$	$0.3 \times 10^{-14}$	$0.1 \times 10^{-14}$
Rep	0.3	$0.7 \times 10^{-14}$	$0.1 \times 10^{-14}$	$0.1 \times 10^{-14}$
	1.0	$0.3 \times 10^{-14}$	$0.1 \times 10^{-14}$	$0.1 \times 10^{-14}$

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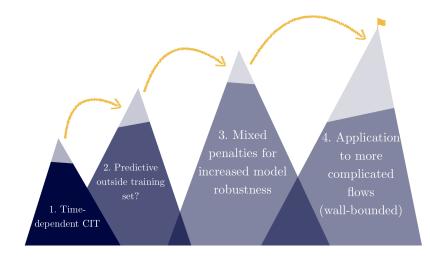
# Sparse Identification uncovers complex dependencies on flow conditions that improve model accuracy.



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Sparse Identification

# Looking ahead





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# **Questions?**



#### This work is supported by the NSF Graduate Research Fellowship Program



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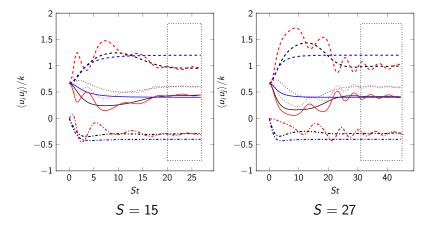
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Fully developed CIT Sparse Identification

Looking ahead

# DNS-generated homogeneous shear turbulence

Comparison of models in the context of the Reynolds-stress equations





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# Sparse identification of fully-developed CIT

$$\underbrace{\frac{\varphi}{\tau_{p}}\left(\langle u_{f}^{'''}u_{p}^{''}\rangle_{p} - \langle u_{f}^{'''2}\rangle_{p}^{1/2}}_{\text{DE}} = \frac{\varphi}{\tau_{p}}\left(\beta_{fp,1}\langle u_{f}^{'''2}\rangle_{f}^{1/2}\langle u_{p}^{''2}\rangle_{p}^{1/2} - \beta_{f,1}\langle u_{f}^{'''2}\rangle_{f}\right)$$
  
Exact expression Existing Closure  
Closure Discovered by Sparse Regression  

$$= 9.1\frac{\varphi_{f}}{k_{f}}\langle u_{f}^{'''2}\rangle - \frac{\varphi}{\tau_{p}}\left((0.5 + 1.9\langle \alpha_{p}\rangle + 0.05Re_{p})\langle u_{f}^{'''2}\rangle + 0.1\langle v_{f}^{'''2}\rangle\right)$$
  

$$+ \frac{\varphi}{\tau_{p}}\left((0.6 - 0.05Re_{p})\langle u_{p}^{''2}\rangle_{p} - 0.5\langle v_{p}^{''2}\rangle_{p}\right) - 0.4Re_{p}\frac{\varphi}{\tau_{p}}\langle u_{f}^{'''2}\rangle_{p}^{\frac{1}{2}}\langle u_{p}^{''2}\rangle_{p}^{\frac{1}{2}}$$

Existing Model Error

0				
			$\langle \alpha_p \rangle$	
		0.001	0.01	0.1
	0.1	0.24	0.05	1.23
$Re_p$	0.3	0.72	0.21	0.32
	1.0	0.35	0.25	0.24

Sparse Identification Error

			$\langle \alpha_p \rangle$	
		0.001	0.01	0.1
	0.1	$0.6 \times 10^{-14}$	$0.2 \times 10^{-14}$	$0.2 \times 10^{-14}$
Rep	0.3	$4.9 \times 10^{-14}$	$0.2 \times 10^{-14}$	$0.4 \times 10^{-14}$
	1.0	$0.4 \times 10^{-14}$	$0.8 \times 10^{-14}$	$0.5 \times 10^{-14}$

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# Sparse identification of fully-developed CIT

$$\underbrace{\frac{\varphi}{\tau_p} \langle u_f'' \rangle_p \langle u_p \rangle_p}_{\text{DP}} = \frac{\varphi}{\tau_p} C_g \langle u_p \rangle_p^2$$
  
Exact expression Existing Closure

Closure Discovered by Sparse Regression

$$= -8.9 \frac{\varepsilon_f}{k_f} \langle u_f^{'''2} \rangle + \frac{\varphi}{\tau_p} \left( (0.6 - 1.9 \langle \alpha_p \rangle - 0.02 Re_p) \langle u_f^{'''2} \rangle + 0.1 \langle v_f^{'''2} \rangle \right) \\ + \frac{\varphi}{\tau_p} \left( 0.7 \langle u_p^{''2} \rangle_p + 0.6 \langle v_p^{''2} \rangle_p \right) - \frac{0.4 Re_p}{\tau_p} \frac{\varphi}{\tau_p} \langle u_f^{'''2} \rangle^{\frac{1}{2}} \langle u_p^{''2} \rangle_p^{\frac{1}{2}}$$

Existing Model Error

	Encound model Encor				
			$\langle \alpha_p \rangle$		
		0.001	0.01	0.1	
	0.1	0.98	0.98	0.96	
$Re_p$	0.3	0.97	0.98	0.95	
-	1.0	1.07	0.86	0.96	

Sparse Identification Error

			$\langle \alpha_p \rangle$	
		0.001	0.01	0.1
	0.1	$1.5 \times 10^{-14}$	$0.2 \times 10^{-14}$	$0.04 \times 10^{-14}$
Rep	0.3	$2.2 \times 10^{-14}$	$0.1 \times 10^{-14}$	$0.01 \times 10^{-14}$
	1.0	$0.3 \times 10^{-14}$	$0.2 \times 10^{-14}$	$0.02 \times 10^{-14}$

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# Homogeneous shear turbulence

The exact Reynolds-Stress equations for shear turbulence<sup>7</sup> are

$$\frac{d}{dt}\langle u_i u_j \rangle = \mathcal{P}_{ij} + \mathcal{R}_{ij} - \frac{2}{3}\varepsilon \delta_{ij}$$

where

- $\mathcal{P}_{ii}$  production of TKE
- $\mathcal{R}_{ii}$  pressure rate-of-strain (redistribution of TKE)
- $\varepsilon$  dissipation of TKE

and unclosed terms are  $\mathcal{R}_{ii}$  and  $\varepsilon$ .

[7] Pope, S. (2012)



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# Homogeneous shear turbulence

A widely accepted closure for the pressures rate-of-strain term, is the LLR-IP model  $^7$ 

$$\mathcal{R}_{ij} = -C_R \frac{\varepsilon}{k} \left( \langle u_i u_j \rangle - \frac{2}{3} k \delta_{ij} \right) - C_2 \left( \mathcal{P}_{ij} - \frac{2}{3} \mathcal{P} \delta_{ij} \right)$$

with typical values  $C_R = 1.8$  and  $C_2 = 3/5$ .

[7] Pope, S. (2012)



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