Reynolds Stress Closure for Nonequilibrium Effects in Turbulent Flows

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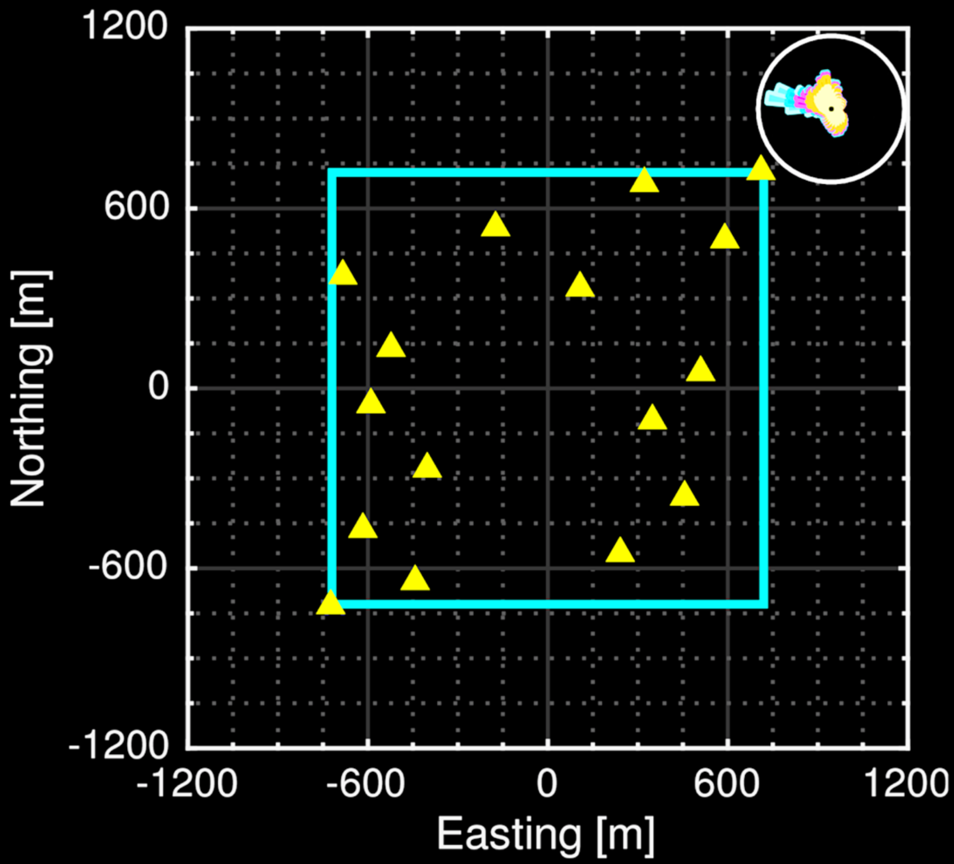
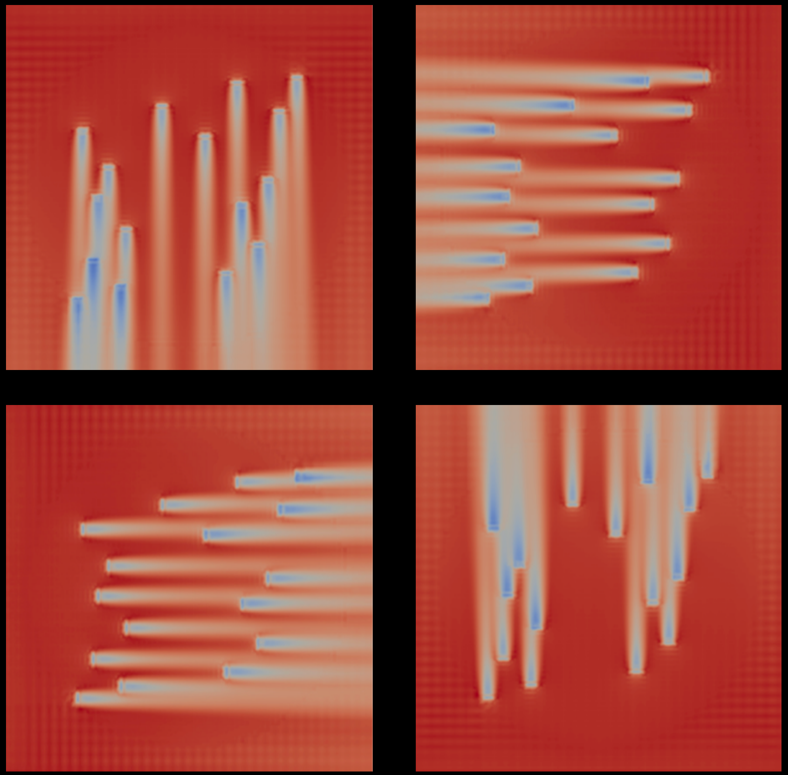
Motivation: Wind Farm Layout Optimization



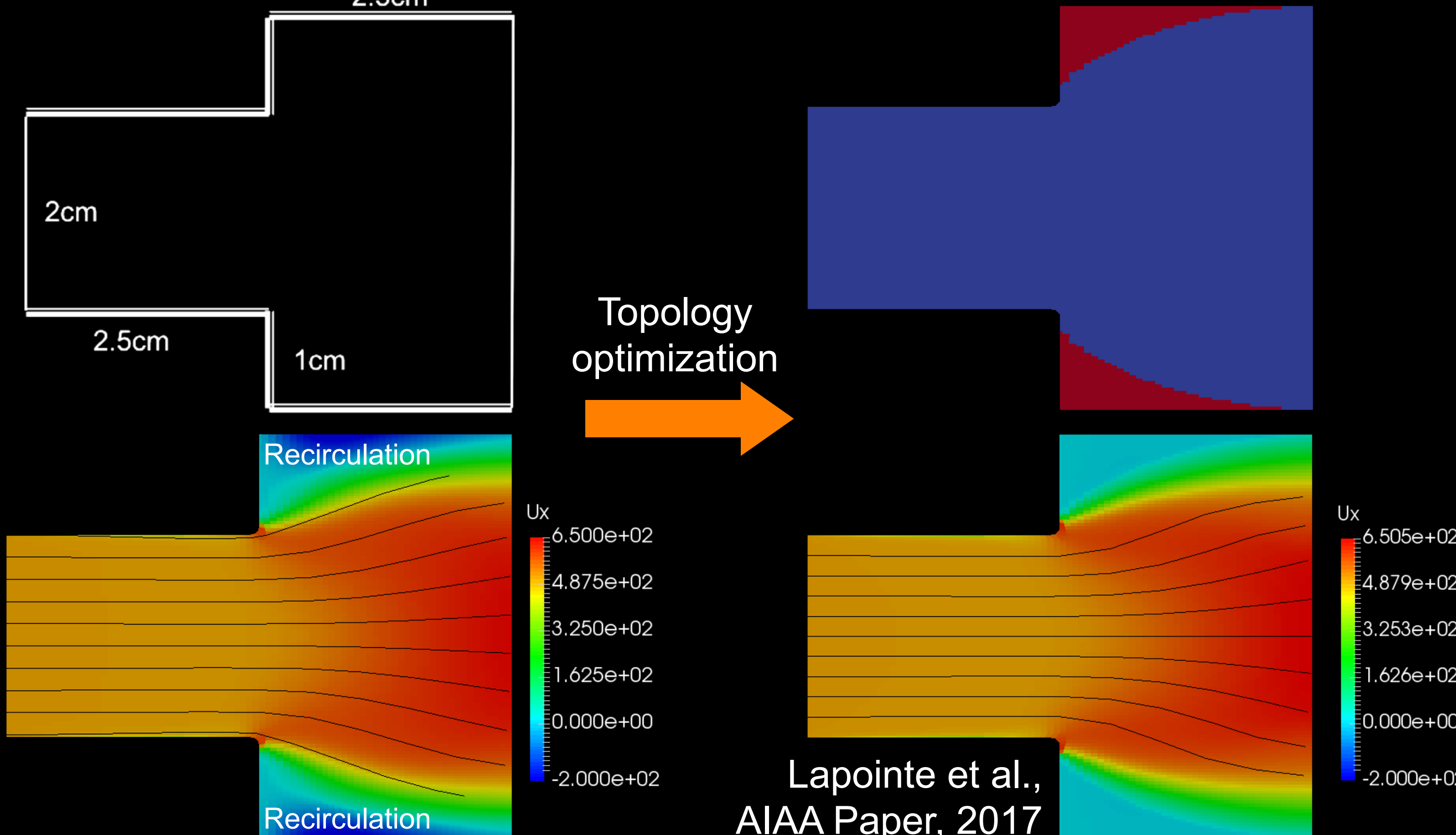


King et al., Wind Energy Sciences, 2017

Adjoint optimization of wind-farm layout using mixing length RANS model

→ How do we account for dynamically varying winds and control?

Motivation: Compressible Flow Optimization



Adjoint optimization (remove recirculation) in supersonic flow using SST k-ω

→ How do we model thrust vectoring, shock-turbulence interactions, etc.?

Challenge: Nonequilibrium Flow Effects

- Many commonly-used RANS models are inaccurate in complex flows, which will pose contin issues as RANS is used for optimization, uncertainty quantification, reduced order modeling etc.

- **Nonequilibrium:** Large variations in flow quantities relative to straining time scale (~1/S) and turbulence response time scale (~k/ε)
  - Anisotropy is not in equilibrium with local instantaneous strain rate

$$\frac{\partial \overline{u}_i}{\partial x_i} = 0$$

$$\frac{D\overline{u}_i}{Dt} = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[2\nu \overline{S}_{ij} - \boxed{\overline{u_i' u_j'}}\right] \qquad \overline{S}_{ij} = \frac{1}{2}\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right)$$

$$\overline{u_i' u_j'} = \frac{2}{3}k\delta_{ij} - \left(\overline{u_i' u_j'}\right)_{aniso}$$

$$a_{ij} \equiv -\frac{(\overline{u_i' u_j'})_{aniso}}{k} = \frac{\overline{u_i' u_j'}}{k} - \frac{2}{3}\delta_{ij}$$

Can we find a physically-accurate closure for the anisotropy a_{ij} that can be readily implemented in CFD codes for solving a wide-range of complex flow problems?

Approach: Anisotropy Transport Equation

- The exact equation for the evolution of the anisotropy is known

Relaxation Destruction

Transport

$$\frac{Da_{ij}}{Dt} = -\left(\frac{P}{\epsilon} - 1\right)\frac{\epsilon}{k}a_{ij} + \frac{1}{k}\left[P_{ij} - \frac{2}{3}P\delta_{ij}\right] + \frac{1}{k}\Pi_{ij} - \frac{1}{k}\left[\epsilon_{ij} - \frac{2}{3}\epsilon\delta_{ij}\right] + \frac{1}{k}\left[D_{ij} - \left(a_{ij} + \frac{2}{3}\delta_{ij}\right)D\right]$$

Lagrangian variations (nonequilibrium) Production Redistribution (pressure-strain)

- Production can be expanded exactly in terms of a_{ij}, S_{ij}, and W_{ij}

$$\left[P_{ij} - \frac{2}{3}P\delta_{ij}\right] = -\frac{4}{3}k\overline{S}_{ij} - k\left(a_{il}\overline{S}_{lj} + \overline{S}_{il}a_{lj} - \frac{2}{3}a_{nl}\overline{S}_{nl}\delta_{ij}\right) + k\left(a_{il}\overline{W}_{lj} - \overline{W}_{il}a_{lj}\right)$$

- This gives the exact anisotropy transport equation that must be solved

$$\frac{Da_{ij}}{Dt} = -\left(\frac{P}{\epsilon} - 1\right)\frac{\epsilon}{k}a_{ij} - \frac{4}{3}\overline{S}_{ij} - \left(a_{il}\overline{S}_{lj} + \overline{S}_{il}a_{lj} - \frac{2}{3}a_{nl}\overline{S}_{nl}\delta_{ij}\right)$$
$$+ \left(a_{il}\overline{W}_{lj} - \overline{W}_{il}a_{lj}\right) + \boxed{\frac{1}{k}\Pi_{ij} - \frac{1}{k}\left[\epsilon_{ij} - \frac{2}{3}\epsilon\delta_{ij}\right] + \frac{1}{k}\left[D_{ij} - \left(a_{ij} + \frac{2}{3}\delta_{ij}\right)D\right]}$$

Approach: Modeled Anisotropy Transport

- The standard local modeled anisotropy equation is obtained from exact equation

$$\frac{Da_{ij}}{Dt} = -\left(\frac{P}{\epsilon} - 1\right)\frac{\epsilon}{k}a_{ij} - \frac{4}{3}\overline{S}_{ij} - \left(a_{il}\overline{S}_{lj} + \overline{S}_{il}a_{lj} - \frac{2}{3}a_{nl}\overline{S}_{nl}\delta_{ij}\right)$$
$$+ \left(a_{il}\overline{W}_{lj} - \overline{W}_{il}a_{lj}\right) + \boxed{\frac{1}{k}\Pi_{ij}} - \frac{1}{k}\cancel{\left[\epsilon_{ij} - \frac{2}{3}\epsilon\delta_{ij}\right]} + \boxed{\frac{1}{k}\left[D_{ij} - \left(a_{ij} + \frac{2}{3}\delta_{ij}\right)D\right]}$$

Primary nonlocal term; usually modeled in terms of purely local variables, a_{ij}, S_{ij}, W_{ij} [e.g. LRR (1975), SSG models (1991)]

High-Re Isotropy

$$\frac{Da_{ij}}{Dt} = -\alpha_1\frac{\epsilon}{k}a_{ij} + \alpha_2\overline{S}_{ij} + \alpha_3\left(a_{il}\overline{S}_{lj} + \overline{S}_{il}a_{lj} - \frac{2}{3}a_{nl}\overline{S}_{nl}\delta_{ij}\right)$$
$$- \alpha_4\left(a_{il}\overline{W}_{lj} - \overline{W}_{il}a_{lj}\right) + \frac{1}{k}\left[D_{ij} - \left(a_{ij} + \frac{2}{3}\delta_{ij}\right)D\right]$$

$$\alpha_1 = \frac{P}{\epsilon} - 1 + C_1, \quad \alpha_2 = C_2 - \frac{4}{3}, \quad \alpha_3 = C_3 - 1, \quad \alpha_4 = C_4 - 1$$

Approach: Prior Anisotropy Models

- Reynolds stress transport models (e.g. LRR, SSG): involve the full solution of the six coupled partial differential equations

$$\frac{Da_{ij}}{Dt} = \boxed{- \alpha_1 \frac{\epsilon}{k} a_{ij} + \alpha_2 \overline{S}_{ij}} + \alpha_3 \left(a_{il}\overline{S}_{lj} + \overline{S}_{il} a_{lj} - \frac{2}{3} a_{nl} \overline{S}_{nl} \delta_{ij} \right) - \alpha_4 \left(a_{il} \overline{W}_{lj} - \overline{W}_{il} a_{lj} \right) + \frac{1}{k} \left[D_{ij} - \left(a_{ij} + \frac{2}{3} \delta_{ij} \right) D \right]$$

- Algebraic stress models (e.g. Gatski and Speziale (1993), Girimaji (1996), Wallin and Johansson(2000): neglect nonequilibrium; retain nonlinearity

$$a_{ij} = G_1 \frac{k}{\epsilon} \overline{S}_{ij} + G_2 \left(\frac{k}{\epsilon} \right)^2 \left[\overline{S}_{il} \overline{S}_{lj} - \frac{\delta_{ij}}{3} \overline{S}_{kl} \overline{S}_{kl} \right] + G_3 \left[\overline{S}_{il} \overline{W}_{lj} - \overline{W}_{il} \overline{S}_{lj} \right]$$

- Boussinesq hypothesis (e.g. k-ε, k-ω, SST): neglect nonequilibrium and nonlinearity

$$a_{ij} = -2 \frac{\nu_T}{k} \overline{S}_{ij}$$

Approach: Nonequilibrium Anisotropy Model

- Instead of just first two terms on RHS, also retain nonequilibrium term on LHS

$$\boxed{\frac{Da_{ij}}{Dt} = \boxed{-\ \alpha_1 \frac{\epsilon}{k} a_{ij} + \alpha_2 \overline{S}_{ij}}}\ - \alpha_3 \left(a_{il}\overline{S}_{lj} + \overline{S}_{il} a_{lj} - \frac{2}{3} a_{nl}\overline{S}_{nl}\delta_{ij} \right)$$
$$-\ \alpha_4 \left(a_{il}\overline{W}_{lj} - \overline{W}_{il} a_{lj} \right) + \frac{1}{k}\left[D_{ij} - \left(a_{ij} + \frac{2}{3}\delta_{ij} \right) D \right]$$

- This yields a simple quasilinear governing equation for the anisotropy

$$\frac{Da_{ij}}{Dt} = -\frac{1}{\Lambda_m} a_{ij} + \alpha_2 \overline{S}_{ij} \qquad \Lambda_m \equiv C_\Lambda \frac{k}{\epsilon}$$

- This simple ODE has an approximate convolution integral solution

$$\boxed{a_{ij}(t) = -2C_\mu \frac{k}{\epsilon} \frac{1}{\Lambda_m(t)} \int_{-\infty}^{t} \overline{S}_{ij}(\tau) e^{-(t-\tau)/\Lambda_m(t)} D\tau}$$

- This solution accounts for nonequilibrium effects and some nonlocality

Approach: Nonequilibrium Model Formulation

- Anisotropy written in terms of an effective strain rate tensor

$$a_{ij} = -2\frac{\nu_T}{k}\widetilde{S}_{ij} \qquad \widetilde{S}_{ij}(t) = \int_{-\infty}^{t} \overline{S}_{ij}(\tau)\frac{e^{-(t-\tau)/\Lambda_m(t)}}{\Lambda_m(t)}D\tau \qquad \Lambda_m \equiv C_\Lambda \frac{k}{\epsilon} \quad C_\Lambda \approx 0.26$$

- Value of C_Λ is constant and determined from nonequilibrium test cases
- In good agreement with previous values of C_Λ

	α_1	C_Λ
Yakhot *et al.* [29]	4.4	0.23
Launder *et al.* [41]	2.4	0.42
Gibson and Launder [42]	2.7	0.37
Gatski and Speziale [5]	4.3	0.23

- Couple to equations for k and ε to find Λ_m

$$\left.\frac{dk}{dt} = -k a_{ij}\overline{S}_{ij} - \epsilon \qquad \frac{d\epsilon}{dt} = -C_{\epsilon 1}\epsilon\, a_{ij}\overline{S}_{ij} - C_{\epsilon 2}\frac{\epsilon^2}{k}\right\}$$

Homogeneous turbulence

- Effective strain evaluated exactly for known straining histories $S_{ij}(t)$
- Homogeneous cases ideal for validation (impulsive shear, periodic shear, etc.)

Results: Impulsively Sheared Turbulence

- LES data of impulsively sheared turbulence from Bardina et al. (1983)
- Boussinesq model predicts immediate increase in turbulence kinetic energy

$$P = -k\, a_{ij}\overline{S}_{ij}$$

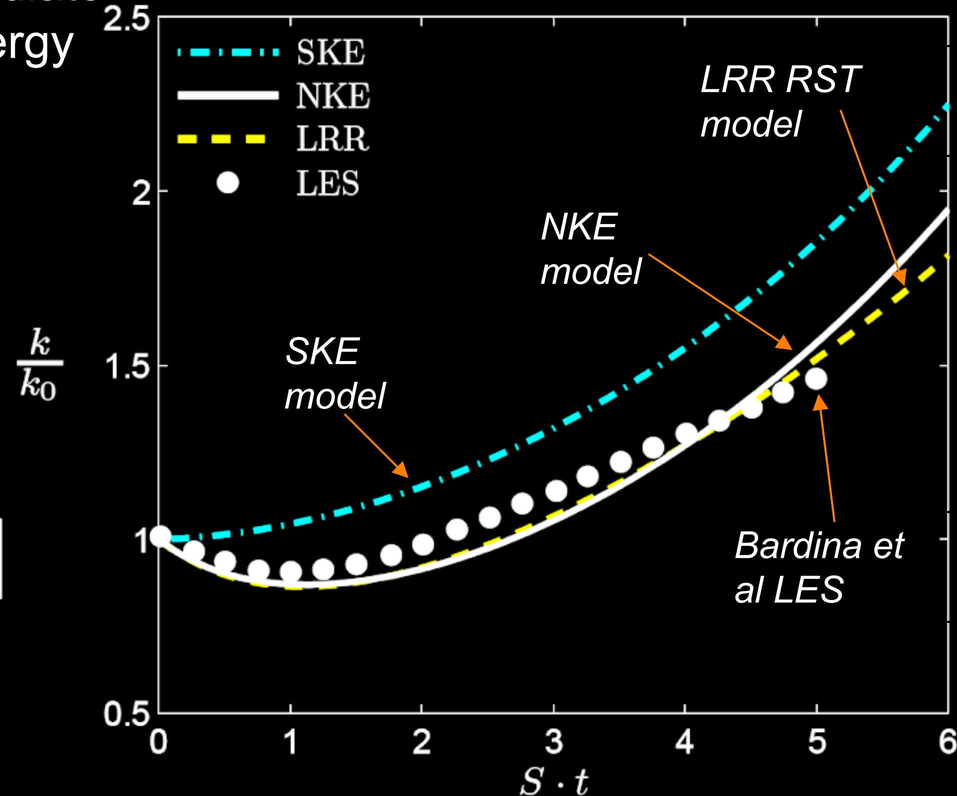
$$a_{12}(t) = a_{21}(t) = -\frac{\nu_T}{k} S$$

- Nonequilibrium model correctly predicts initial decay

$$a_{12}(t) = a_{21}(t) = -\frac{\nu_T}{k} S \left[1 - e^{-t/\Lambda_m}\right]$$

- Nonequilibrium k lags behind equilibrium k for all times

$$\overline{S}_{12}(t) = \overline{S}_{21}(t) = \begin{cases} 0 & \text{for } t < 0 \\ S/2 & \text{for } t \geq 0 \end{cases}$$

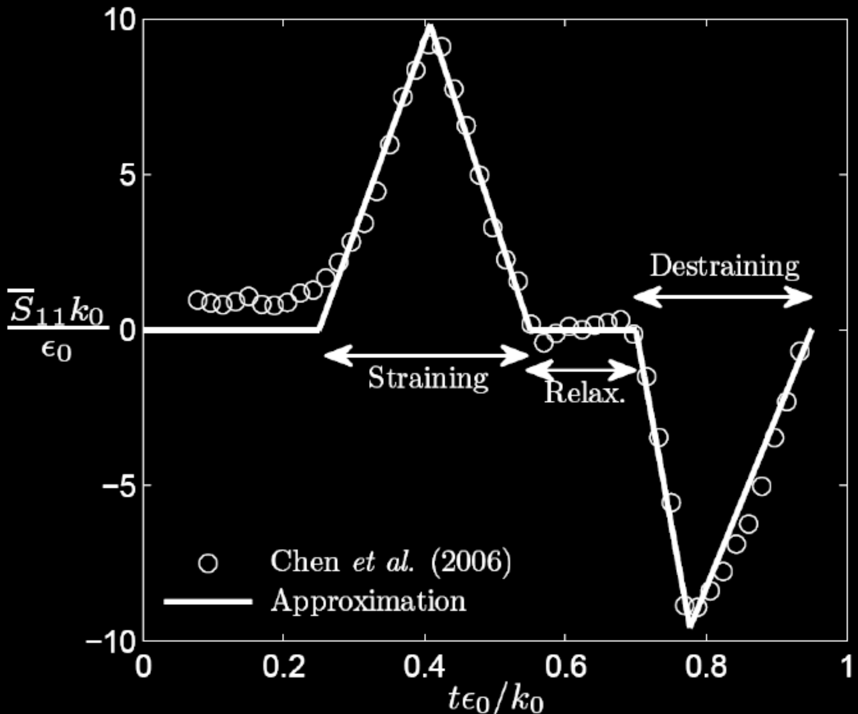


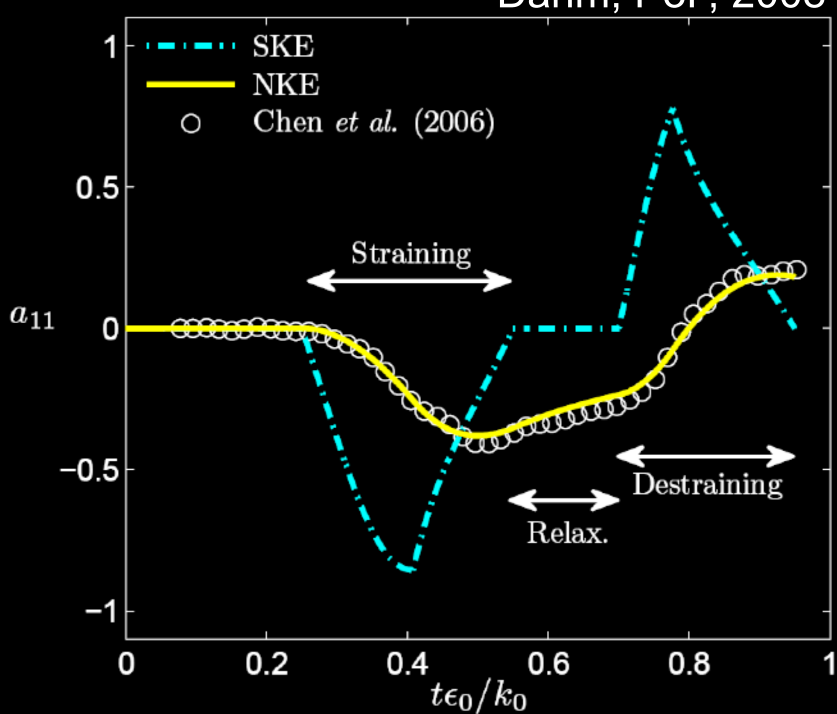
Hamlington & Dahm, PoF, 2008

Results: Piston Driven Turbulence

- Experimental data from Chen, Meneveau, and Katz (2006)
- Equilibrium model predicts large changes in anisotropy during straining and destraining; zero anisotropy during relaxation phase
- Nonequilibrium model correctly predicts gradual changes in anisotropy and nonzero anisotropy during relaxation

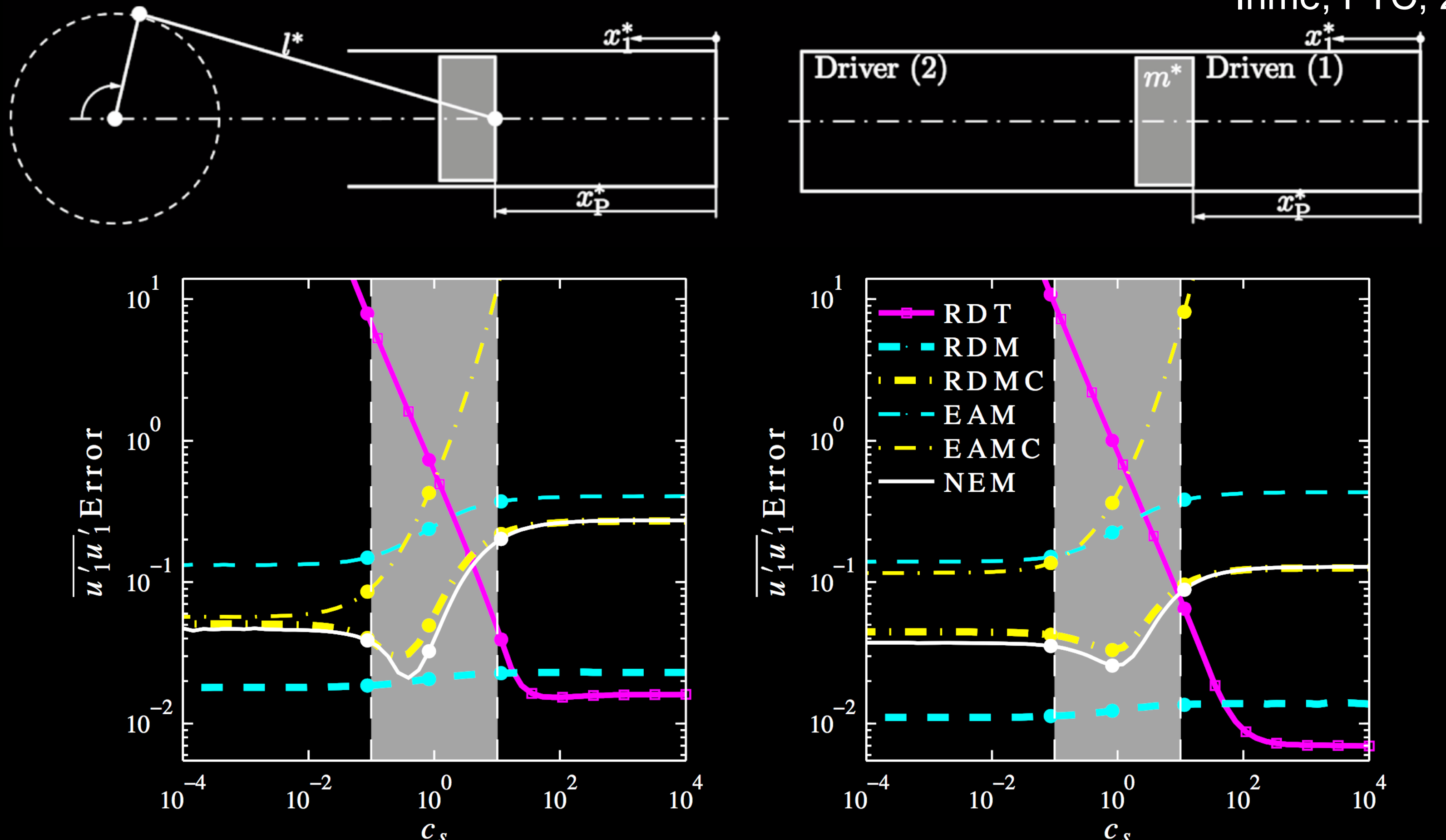
Hamlington & Dahm, PoF, 2008





Results: IC Engine and RCM

Hamlington & Ihme, FTC, 2014

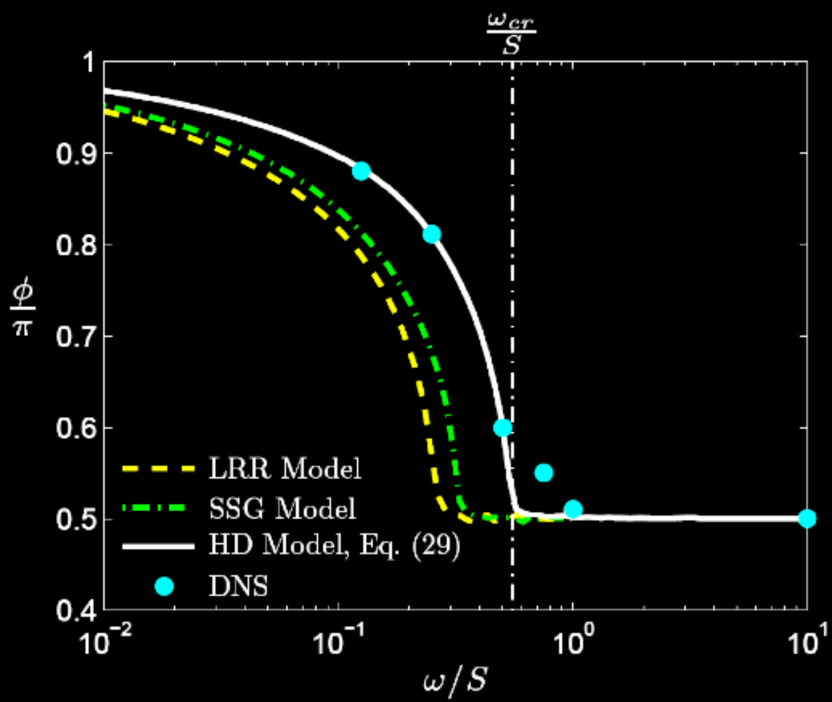


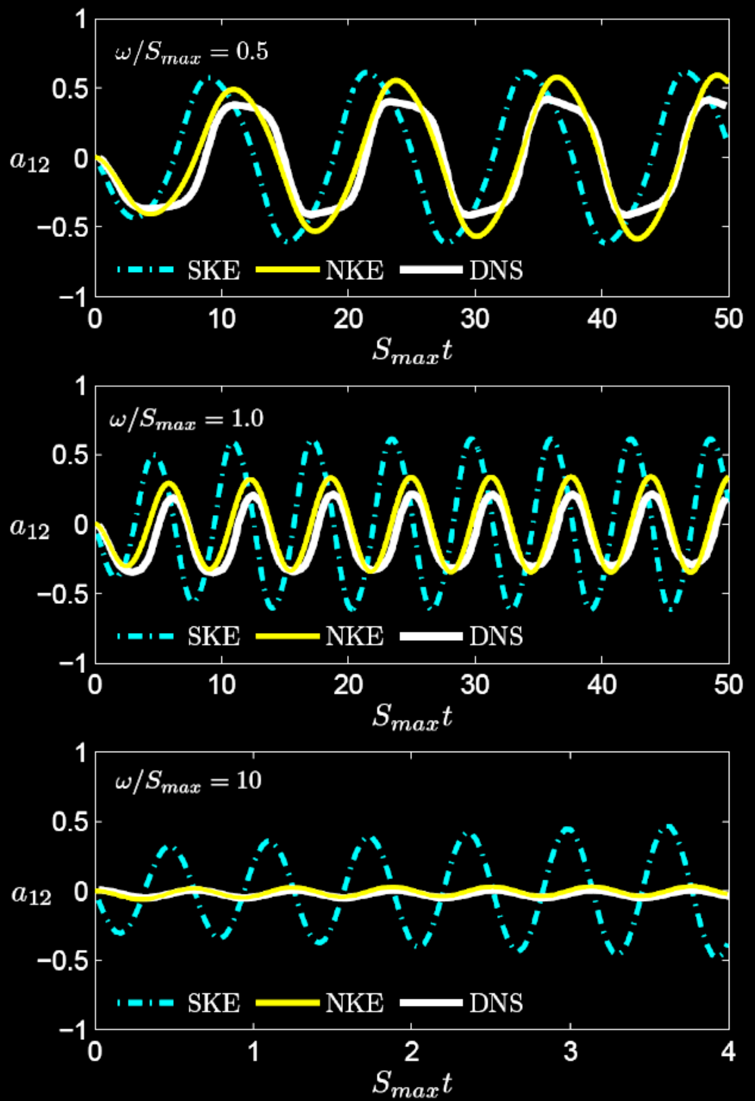
(a) Internal combustion engine.

(b) Rapid compression machine.

Results: Periodically Sheared Turbulence

- DNS data from Yu and Girimaji (2006)
- Equilibrium model predicts anisotropy and shear in phase; over-predicts amplitude
- Nonequilibrium model predicts correct phase and decreasing amplitude with increasing shearing frequency





Approach: Time-Local Model Formulation

- Nonequilibrium turbulence anisotropy relation

$$a_{ij}(t) = -2C_\mu \frac{k}{\epsilon}\widetilde{S}_{ij}(t) \qquad \widetilde{S}_{ij}(t) = \int_{-\infty}^{t} \overline{S}_{ij}(\tau)\frac{e^{-(t-\tau)/\Lambda_m(t)}}{\Lambda_m(t)}D\tau$$

- Time-expansion of strain rate tensor history along mean-flow streamline

$$\overline{S}_{ij}(\tau) = \overline{S}_{ij}(t) - \left.\frac{D\overline{S}_{ij}}{Dt}\right|_t (t-\tau) + \frac{1}{2}\left.\frac{D^2\overline{S}_{ij}}{Dt^2}\right|_t (t-\tau)^2 + \cdots$$

- Substitute in convolution integral for effective strain rate

$$\widetilde{S}_{ij}(t) = \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\left.\frac{D^n\overline{S}_{ij}}{Dt^n}\right|_t \int_{-\infty}^{t}(t-\tau)^n\frac{e^{-(t-\tau)/\Lambda_m}}{\Lambda_m}D\tau$$

- Provides exact time-local form of effective strain rate tensor

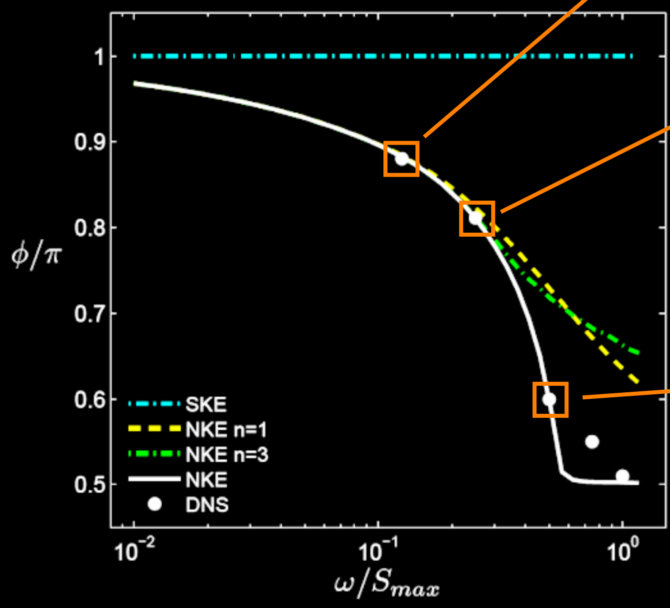
$$\widetilde{S}_{ij} = \overline{S}_{ij} + \sum_{n=1}^{\infty}(-\Lambda_m)^n\left.\frac{D^n\overline{S}_{ij}}{Dt^n}\right|_t \qquad \Lambda_m \equiv C_\Lambda\frac{k}{\epsilon} \qquad C_\Lambda \approx 0.26$$

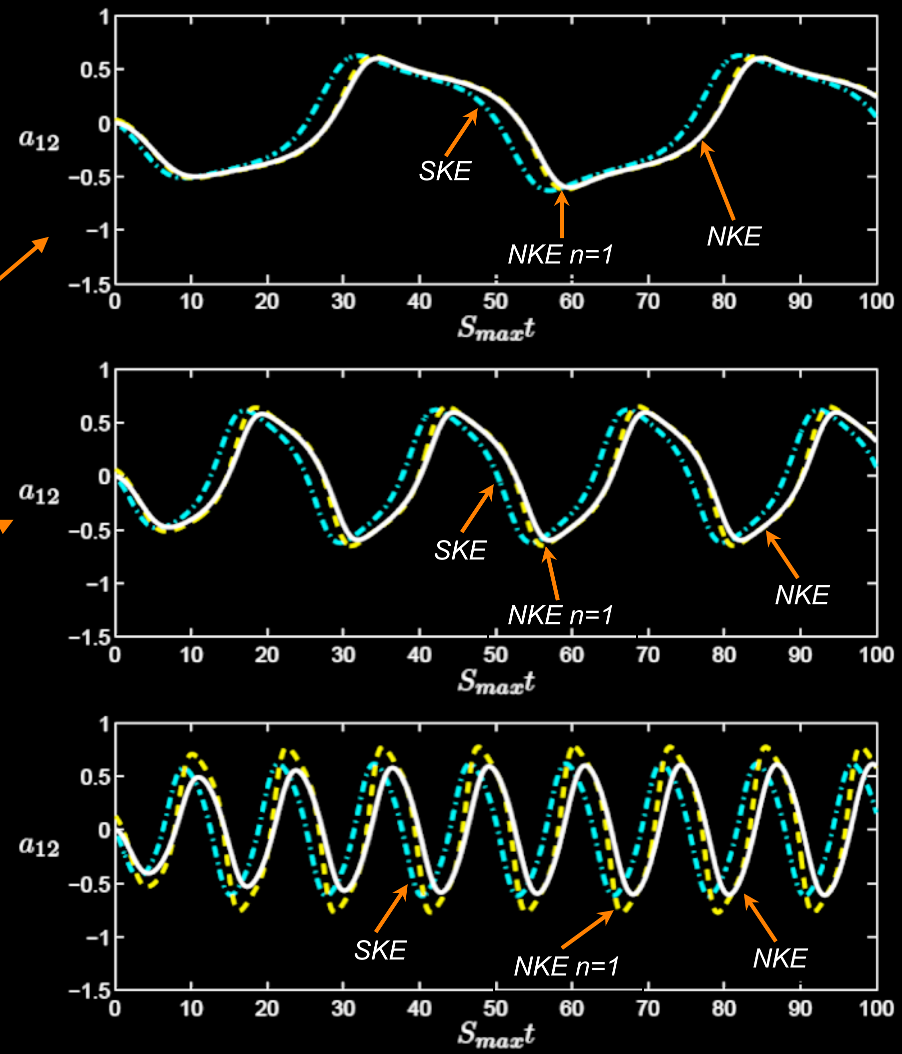
Results: Time-Local Periodic Shear

$$a_{ij}(t) = -2C_\mu \frac{k}{\epsilon} \widetilde{S}_{ij}(t)$$

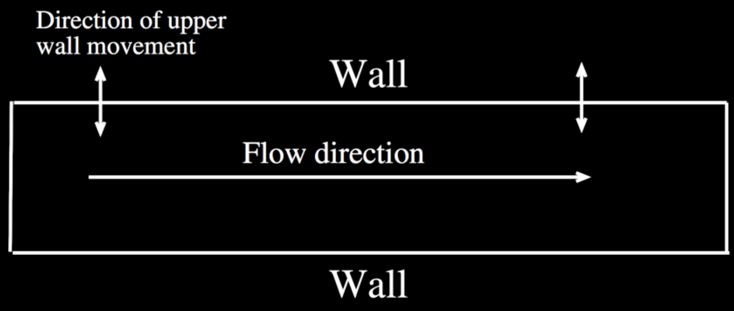
$$\widetilde{S}_{ij} = \overline{S}_{ij} + \sum_{n=1}^{\infty} (-\Lambda_m)^n \left. \frac{D^n \overline{S}_{ij}}{Dt^n} \right|_t$$

$$\Lambda_m \equiv C_\Lambda \frac{k}{\epsilon} \qquad C_\Lambda \approx 0.26$$

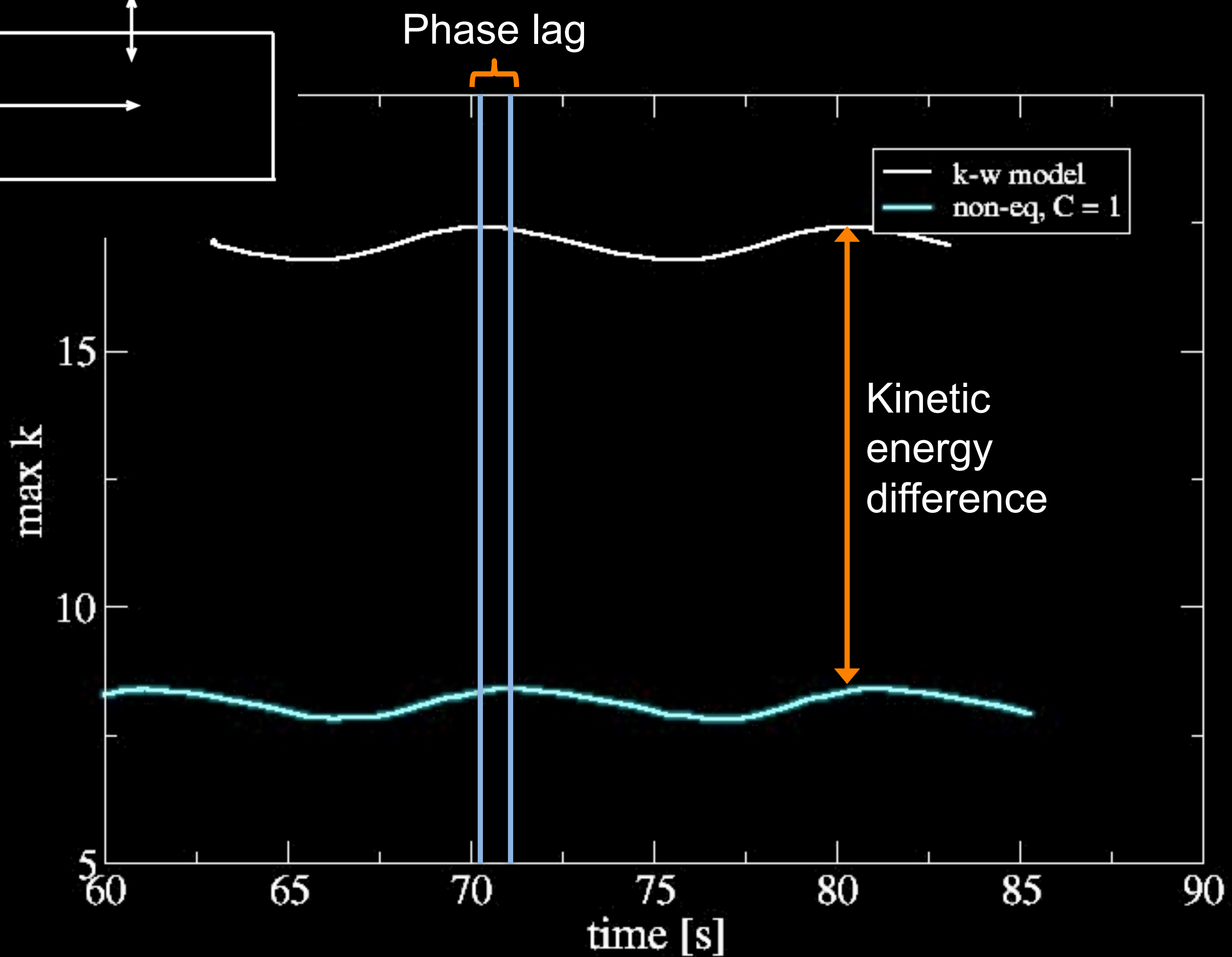




Results: Oscillating Channel



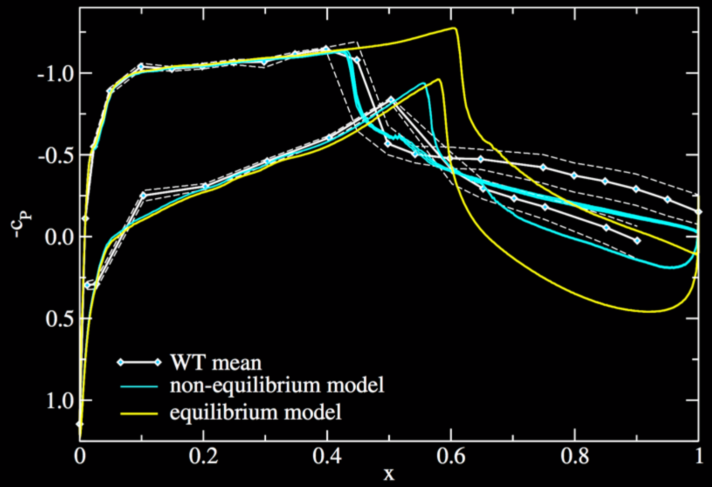
$$\Delta y = 0.25H\sin(2\pi f t)$$

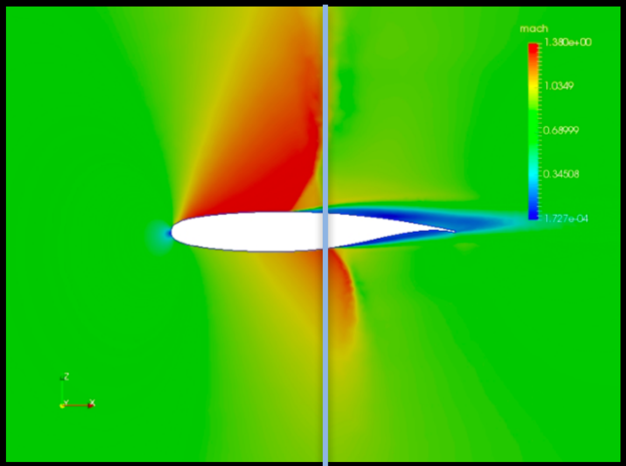


Jirasek et al., AIAA Paper, 2018

Results: Benchmark Supercritical Wing

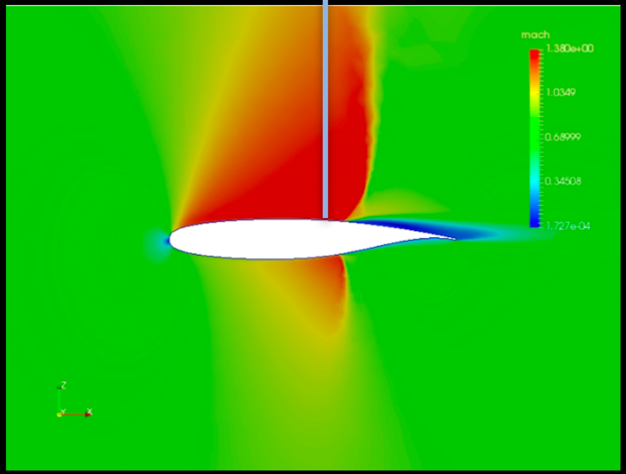
Heeg & Piatak, AIAA Paper, 2013





Equilibrium k-ω model

Shift in shock location

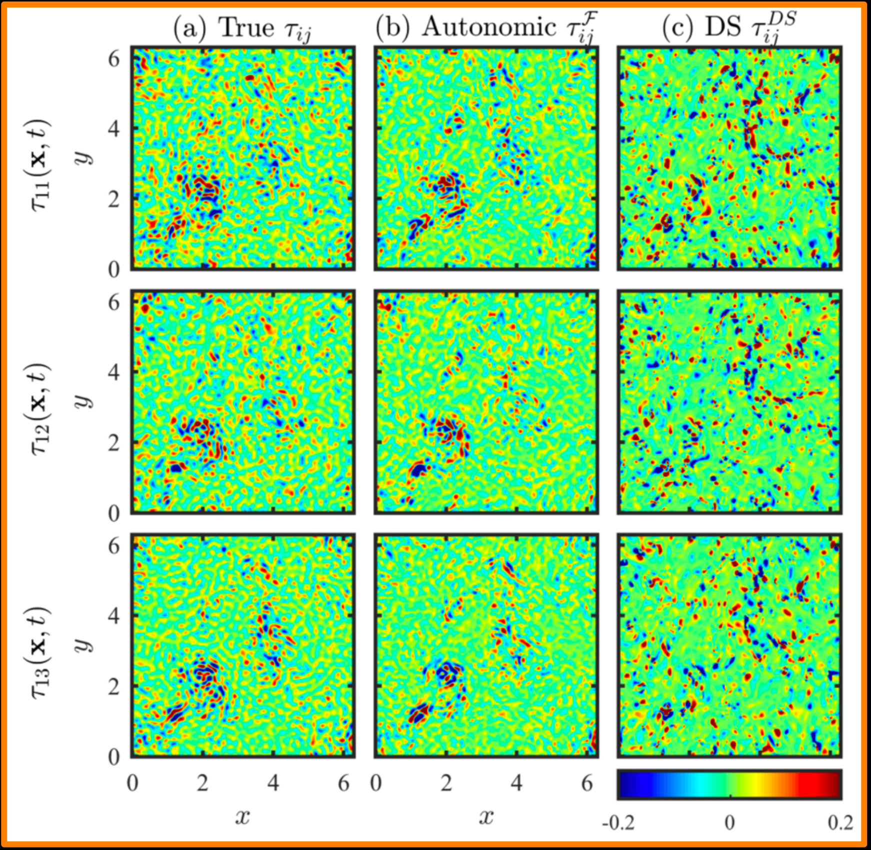


Nonequilibrium k-ω model

Jirasek et al., AIAA Paper, 2018

Outlook

- This has been a “physics based” approach to modeling
- Data-driven approaches have the potential to provide new model formulations and enhanced accuracy
- Sometimes data driven approaches are “physics agnostic” (e.g., autonomic closure for LES)
- Is there a way to combine a high-DOF physics based model (e.g., from anisotropy transport equation) with a data driven approach?



King, Hamlington & Dahm, PRE, 2016

$$\overline{u_i'u_j'} = \frac{2}{3}k\delta_{ij} - 2\nu_T\widetilde{S}_{ij}$$

$$\widetilde{S}_{ij} = \overline{S}_{ij} + \sum_{n=2}^{\infty}\frac{C_2^{(n)}}{\alpha_2}\Lambda^{2n-2}\left(\nabla^2\right)^{n-1}\overline{S}_{ij} + \sum_{n=1}^{\infty}(-\Lambda_m)^n\frac{D^n\overline{S}_{ij}}{Dt^n}$$