Single-point second-moment turbulence models – why, where and where not

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The holy grail

We are promised a 'model-free' CFD world

A Boeing 747 is not a homogeneous square box!



Hybrid LES-RANS

Courtesy: ANSYS, Germany

- > Mean-flow scales: t, ℓ
- > Kolmogorov scales: τ , η
- > Ratios: $t / \tau \sim Re^{1/2}, \ell / \eta \sim Re^{3/4}$
- > Grid: $N_{\eta} \sim R e^{9/4}$

- Aircraft: $Re \square 10^8$
- Nodes: $N_n \square 10^{19}$
- Time steps: $N_{\tau} \Box 10^6 10^7$
- Current estimate of time of realisation: 2080
- Current estimate for LES: 2045 (based on resolution at Taylor scale)
- Current capability: RANS and RANS-LES hybrids
- 95%+ of all engineering CFD is based on RANS

The cost

- Mesh: 10¹⁹
- Cost: 5000 CPU years per 1 second of flying at 1Tflop throughput



- Model-free DNS used to
 - > investigate fundamental physics;
 - > examine subgrid-scale models (a-priori testing)
 - > Develop, calibrate and validate RANS models
- Largest channel-flow DNS: $Re_{\tau} = 964$, 2.7x10⁹ nodes (Del Alamo et al, 2004)
- Example: insight into origin of drag reduction by spanwise wall oscillation (Touber & Leschziner, 2010)
 Travelling
 - $ightarrow Re_{\tau} = 500 (\rightarrow 1000)$
 - Drag reduction up to 40%
 - > 0.5x10⁹ nodes, 1M CPU hours



Fundamental mechanism of streak response

- Streak formation and re-orientation mechanisms
- Conditional sampling and averaging
- Decomposition of small streaks/super-streaks

Streak decay, regeneration,

- Modulation mechanisms
- Linear analysis (GOP)



Reduction of wall-normal fluctuations around streaks in % due to actuation





> Requires closure equations for the periodic and stochastic terms: too complex in practice – URANS use RANS models + $\partial/\partial t$

Reynolds stresses related to known or determinable quantities: 0

 $\overline{u_{i}u_{j}} = f_{ij} \begin{pmatrix} S_{ij}, \Omega_{ij}, S_{kl}S_{kl}, \Omega_{kl}\Omega_{kl}, \\ \text{length-scale surrogates} \\ \text{turbulence invariates} \end{pmatrix} \qquad S_{ij} \text{ Strain tensor} \\ \Omega_{ij} \text{ Vorticity tensor}$

- Ultimately, need to relate to stresses and mean velocity. •
- Modelling principles not only "ad-hoc curve fitting" ٩
 - strong fundamental foundation;
 - \succ resolution of anisotropy;
 - correct response to shear and normal straining;
 - correct response to curvature and body forces;
 - frame-invariance ("objectivity");
 - \succ realisability;
 - correct approach to 2-component turbulence at wall and fluid-fluid interfaces;
 - satisfactory numerical stability;
 - economy.

 About 150 models & major variations, many meant for restricted flow classes



Defects of linear eddy-viscosity models

- Linear EVM:
 - Well suited to thin shear flow
 - Much less well suited to separated and highly 3d flow
 - No resolution of anisotropy
 - Wrong sensitivity to flow curvature, rotation, normal straining and body forces
 - Reliant on ad-hoc corrections
- Defects are rooted in
 - Inapplicability of linear stress-strain relations
 - Isotropic nature of viscosity, relating to scalar turbulence properties
 - Calibration by reference to simple, near-equilibrium flows
 - Excessive extrapolation to complex condition.
- Only fundamentally credible alternative
 - Modelling based on exact equations for the Reynolds stresses
 - Strong resistance from engineering community complexity

Reynolds-Stress-Transport Modelling

- Introduce the Reynolds decomposition $U_i = \overline{U}_i + u_i$ etc. into the NS equations.
- Subtract from this the corresponding RANS equation.
- Repeating the above, but with the indices *i* and *j* interchanged.
- Add the two equations.
- Time-averaging the result:



> C_{ij} , P_{ij} , F_{ij} , Φ_{ij} , ε_{ij} and d_{ij} represent, respectively, stress convection, production by strain, production by body forces (e.g. buoyancy), dissipation, pressure-strain redistribution and diffusion

The Argument for resolving anisotropy

- Production is a key process: it drives the stresses.
- It requires no approximations if stresses and velocity are known
- It is reasonable to assume, tentatively:

Stress = Production x Time (*capital* = *interest rate x time*)

• Exact equations imply complex stress-strain linkage

$$\rho \overline{u_i u}_j \longleftrightarrow -\tau \left\{ \underbrace{\overline{u_i u_k}}_{P_{ij}} \frac{\partial U_j}{\partial x_k} + \underbrace{\overline{u_j u_k}}_{P_{ij}} \frac{\partial U_i}{\partial x_k} \right\} + \tau \times Body \text{-force production}$$

- Hence, simple EVM stress-strain linkage is inapplicable
- Analogous linkage between scalar fluxes and production

$$\rho \overline{u_i \varphi} \longleftrightarrow - \tau_{\varphi} \left\{ \overline{u_i u_k} \frac{\partial \Phi}{\partial x_k} + \overline{u_i \varphi} \frac{\partial U_i}{\partial x_k} \right\} + \tau_{\varphi} \times Body \text{-force production}$$

• Hence, Fourier-Fick law (eddy-diffusivity approximation) $\rho \overline{u_i \varphi} = -\frac{\mu_i}{\sigma_{\varphi}} \frac{\partial \Psi}{\partial x_i}$ not valid • Only one shear strain, only one shear stress

$$\frac{D\overline{uv}}{Dt} = -\overline{v^2} \frac{\partial \overline{U}}{\partial y} + \overline{p} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) - \frac{\partial}{\partial y} \left(\overline{uv^2} + \overline{pu} \right) + \frac{\mu}{\rho} \frac{\partial \overline{uv}}{\partial y} - \varepsilon_{12}$$

$$\frac{D\overline{u^2}}{Dt} \neq -2\overline{uv} \frac{\partial \overline{U}}{\partial y} + 2\frac{p}{\rho} \frac{\partial u}{\partial x} - \frac{\partial}{\partial y} \left(\overline{u^2v} \right) + 2\frac{\mu}{\rho} \frac{\partial \overline{u^2}}{\partial y} - \varepsilon_{11}$$

$$\frac{D\overline{v^2}}{Dt} = 0 + 2\frac{p}{\rho} \frac{\partial v}{\partial y} - \frac{\partial}{\partial y} \left(\overline{v^3} + \frac{2\overline{pv}}{\rho} \right) + 2\frac{\mu}{\rho} \frac{\partial \overline{v^2}}{\partial y} - \varepsilon_{22}$$

$$\sum = 0 + 2\frac{p}{\rho} \frac{\partial w}{\partial y} - \frac{\partial}{\partial x} \left(\overline{vw^2} \right) + 2\frac{\mu}{\rho} \frac{\partial \overline{w^2}}{\partial y} - \varepsilon_{33}$$
Anisotropy
$$\sum = 0 + 2\frac{p}{\rho} \frac{\partial w}{\partial x} - \frac{\partial}{\partial x} \left(\overline{vw^2} \right) + 2\frac{\mu}{\rho} \frac{\partial \overline{w^2}}{\partial y} - \varepsilon_{33}$$

- Homogeneous shear
 - Development in time of stresses normalized by k
- Channel flow
 - Normal and shear stresses



The importance of anisotropy: expansion (deceleration)



Anisotropy in expansion and contraction





Anisotropy in plain strain





- Inapplicability of Fourier-Fick law in scalar transport
 - Production of flux vector:

$$P_{u_i\phi} = -\overline{u_i u_k} \frac{\partial \Phi}{\partial x_k} - \overline{u_i \varphi} \frac{\partial U_i}{\partial x_k}$$

Reynolds-Stress-Transport Modelling

• Closure of exact stress-transport equations

$$\frac{D\overline{u_{i}u_{j}}}{Dt} = -\left\{ \overline{u_{i}u_{k}} \frac{\partial U_{j}}{\partial x_{k}} + \overline{u_{j}u_{k}} \frac{\partial U_{i}}{\partial x_{k}} \right\} + (Pressure - velocity)$$

$$C_{ij} = Advective Transport$$

$$P_{ij} = Production$$

+ Diffusion – Dissipation

- Pressure-velocity, dissipation and diffusion require approximation
- About 10-15 major closures forms
- Modern closure aims at realisability, 2-component limit, coping with strong inhomogeneity and compressibility
- Additional equations for dissipation tensor \mathcal{E}_{ii}
- At least 7 pde's in 3D (up to 17 in heat/scalar transport)
- Numerically difficult in complex geometries and flow
- Can be costly
- Dissipation and pressure-velocity are major sources of error

The exact dissipation-rate equation

 $\mathbf{D}\varepsilon$ $\partial U_k \varepsilon$ $\partial \varepsilon$ $\overline{\mathbf{D}t}$ ∂t ∂x_k C_{ε} $\partial u_i \partial u_k$ $\frac{\partial u_l}{\partial x_i} \frac{\partial u_l}{\partial x_k}$ $\partial^2 U_i$ ∂U_i ∂u_i $-2\nu u_k \overline{\partial x_l} \overline{\partial x_k \partial x_l}$ $\partial x_l \partial x_l$ ∂x_k P_{ϵ}^3 $P_{\epsilon}^1 + P_{\epsilon}^2$ 2 $\partial^2 u_i$ $\partial u_i \, \partial u_i \, \partial u_k$ $-2\nu \frac{\partial x_k}{\partial x_k} \frac{\partial x_l}{\partial x_l} \frac{\partial x_l}{\partial x_l}$ $\partial x_k \partial x_l$ P_{ε}^4 Y $\partial \varepsilon$ д д 2ν dur $-\overline{u_k\varepsilon})$ + ∂x_k $\overline{\partial x_k}$ ∂x_k $\partial x_i \partial x_i$ ∂x_k $\mathcal{D}_{\epsilon}^{t}$ $\mathcal{D}^p_{arepsilon}$ $\mathcal{D}_{\varepsilon}^{\nu}$ \mathcal{D}_{ϵ}

Modelled dissipation-rate equation



- In energy equilibrium, $P_k = \varepsilon$, and the imbalance is absorbs by diffusion
- Transport equations for \mathcal{E}_{ii} are too complex as basis for modelling
- Anisotropy in dissipation algebraic approximations of the form:

$$\varepsilon_{ij} = \underbrace{f_e \frac{2}{3} \varepsilon \delta_{ij}}_{k} + (1 - f_e) \frac{u_i u_j}{k} \varepsilon$$

• In most models, $f_e = 1$ reflecting assumption of small-scale isotropy

- Regarded as least influential (suggested by DNS/LES).
- Represented as gradient-diffusion with tensorial diffusivity.
- Simplest model:

$$Diff_{ij} = -\frac{\partial}{\partial x_k} \left\{ c_d \frac{k}{\varepsilon} \overline{u_k u_m} \frac{\partial \overline{u_j u_j}}{\partial x_m} \right\}$$

- Based on observation that the most important fragment in the exact diffusion term is $\overline{u_k u_i u_j}$.
- It can be shown, via transport equations for triple correlation, $u_k u_i u_j$, that the production of these triple correlations is by gradients of stresses of the form $P_{ijk} = -\overline{u_k u_m} \frac{\partial \overline{u_j u_j}}{\partial x} + \dots$
- Suggests (also on dimensional grounds) $Diff_{ij} = -\frac{\partial}{\partial x_k} \left\{ c(\text{time scale}) \times (\text{production}_{ijk}) \right\}$

Closure – pressure-strain / velocity

- Extremely important: responsible for redistribution among normal stresses. Regarded as the hardest term to model
- Pressure-velocity dictates energy transfer and hence v^2
- But v^2 dictates uv

$$\frac{D\overline{uv}}{Dt} = -\overline{v^2} \frac{\partial \overline{U}}{\partial y} + \overline{\rho} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) - \frac{\partial}{\partial y} \left(\overline{uv^2} + \overline{pu} \right) + \frac{\mu}{\rho} \frac{\partial \overline{uv}}{\partial y} - \varepsilon_{12}$$

$$\frac{D\overline{u^2}}{Dt} = -2\overline{uv} \frac{\partial \overline{U}}{\partial y} + 2\frac{\overline{\rho}}{\rho} \frac{\partial u}{\partial x} + \frac{\partial}{\partial y} \left(\overline{u^2v} \right) + 2\frac{\mu}{\rho} \frac{\partial \overline{u^2}}{\partial y} - \varepsilon_{11}$$

$$\frac{D\overline{v^2}}{Dt} = 0 + \frac{2\overline{\rho}}{\rho} \frac{\partial v}{\partial y} - \frac{\partial}{\partial y} \left(\overline{v^3} + \frac{2\overline{\rho v}}{\rho} \right) + 2\frac{\mu}{\rho} \frac{\partial \overline{v^2}}{\partial y} - \varepsilon_{22}$$

$$\frac{D\overline{w^2}}{Dt} = 0 + \frac{2\overline{\rho}}{\rho} \frac{\partial w}{\partial z} - \frac{\partial}{\partial x} \left(\overline{vw^2} \right) + 2\frac{\mu}{\rho} \frac{\partial \overline{w^2}}{\partial y} - \varepsilon_{33}$$

- Subject to constrains:
 - > Isotropisation: transfer of energy from largest stress to lower ones
 - Inhibition of isotropisation at walls/interfaces (splatting, reflection)
 - shear stresses have to decline as isotropisation progresses
- Guidance provided by 'exact' integration for pressure-fluctuations and substitution in pressure-velocity correlation

$$\Phi_{ij} = \frac{\overline{p}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)}{\left(\frac{\partial u_i}{\partial x_l} + \frac{\partial u_j}{\partial x_j}\right)^* \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)} \frac{dV(\mathbf{x}^*)}{|\mathbf{x} - \mathbf{x}^*|} + \frac{1}{4\pi} \int_{V} \left\{ 2\left(\frac{\partial u_m}{\partial x_l}\right)^* \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \left(\frac{\partial U_l}{\partial x_m}\right)^* \right\} \frac{dV(\mathbf{x}^*)}{|\mathbf{x} - \mathbf{x}^*|} + \frac{1}{8} \text{ body-force and surface terms}}{B_{ijkl}}$$

Closure – pressure-strain

• Suggests the general Ansatz:

$$\Phi_{ij} = \varepsilon A_{ij} \{a_{ij}\} + k B_{ijkl} \{a_{ij}\} \frac{\partial U_k}{\partial x_l} \qquad \left\{a_{ij} \equiv \frac{u_i u_j}{k} - \frac{2}{3}\delta_{ij}\right\}$$

(+body-force and wall terms)

- Most complex model is cubic
- Much more popular is the quasi-linear form

$$\Phi_{ij} = -C_1 \frac{\varepsilon}{k} \left(\overline{u_i u_j} - \frac{2}{3} \delta_{ij} k \right) - C_2 \left(P_{ij} - \frac{2}{3} \delta_{ij} P_k \right)$$

(+body-force and wall terms)

- This is a sink term in the second-moment equations, depressing anisotropy in proportion to anisotropy of stresses and productions
- Ensures that anisotropy in stresses and productions drives energy from above-average normal stresses to below-average ones
- Coefficients sensitized to anisotropy invariants, turbulence Reynolds number....in lieu of non-linear expansions

Closure – pressure-strain

$$\begin{split} \Phi_{IJ1}^{\text{inf}} &= f_{w1} \frac{\tilde{\rho}\tilde{\epsilon}}{\tilde{k}} \left(\tilde{u}_{i}^{v} \tilde{u}_{k}^{w} d_{i}^{A} d_{k}^{A} \delta_{ij} - \frac{3}{2} \tilde{u}_{i}^{v} \tilde{u}_{k}^{w} d_{j}^{A} d_{k}^{A} - \frac{3}{2} \tilde{u}_{j}^{v} \tilde{u}_{k}^{w} d_{i}^{A} d_{k}^{A} \right) \\ &+ f_{w2} \frac{\tilde{\rho}\tilde{\epsilon}}{\tilde{k}^{2}} \left(\tilde{u}_{m}^{w} \tilde{u}_{m}^{w} \tilde{u}_{m}^{w} \tilde{u}_{m}^{w} \tilde{u}_{n}^{A} d_{i}^{A} \delta_{ij} - \frac{3}{2} \tilde{u}_{i}^{v} \tilde{u}_{m}^{w} \tilde{u}_{m}^{w} \tilde{u}_{i}^{A} d_{j}^{A} d_{k}^{A} \right) \\ &= -\frac{3}{2} \tilde{u}_{j}^{v} \tilde{u}_{m}^{w} \tilde{u}_{m}^{w} \tilde{u}_{i}^{w} d_{i}^{A} d_{i}^{A} \right) \\ &= \frac{3}{2} \tilde{u}_{ij}^{v} \tilde{u}_{m}^{w} \tilde{u}_{m}^{w} \tilde{u}_{i}^{w} d_{i}^{A} d_{i}^{A} \right) \\ &= \frac{3}{2} \tilde{u}_{ij}^{v} \tilde{u}_{m}^{w} \tilde{u}_{m}^{w} \tilde{u}_{i}^{w} d_{i}^{A} d_{i}^{A} d_{i}^{A} \right) \\ &= \frac{3}{2} \tilde{u}_{ij}^{v} \tilde{u}_{m}^{w} \tilde{u}_{m}^{w} \tilde{u}_{i}^{w} d_{i}^{A} d_{i}^{A} d_{i}^{A} \\ &= \frac{3}{2} \tilde{u}_{ij}^{v} \tilde{u}_{m}^{w} \tilde{u}_{m}^{w} \tilde{u}_{i}^{w} d_{i}^{A} d_{i}^{A} d_{i}^{A} \right) \\ &= \frac{3}{2} \tilde{u}_{ij}^{v} \tilde{u}_{m}^{w} \tilde{u}_{m}^{w} \tilde{u}_{i}^{w} d_{i}^{A} d_{i$$

- Construction and calibration rely heavily on highly-resolved experimental & simulation data
- Done mostly by reference to thin-shear-flow data
- Models work well for many flows
- Notable exception: flow separating from curved surfaces (2d & 3d)
- Associated with dynamics of highly unsteady separation (& preseparation)



Separation from curved surface



- Model defects are difficult to cure, but efforts are ongoing
- Example: re-examination of dissipation and pressure-velocity interaction terms in separation from curved ramp
- Foundation: highly-resolved simulation near DNS, 25M nodes



- Re_{H} =13700; Re_{Θ} = 1150
- Second moments, invariants, budgets of all second moments....
- Part of larger study on separation control with synthetic jets
- Experimental data



Starting point

Choice of basic model, based on full computation





Defect identification

Budgets for *uv* and *uu* •



Model fragmentation - dissipation

- A-priori study of dissipation-rate equation
- Isolated solution of equation
- LES strains and stresses input into equation
- Only output is dissipation
- Examination of a range of corrections in efforts to procure agreement with LES data for dissipation rate



Model fragmentation - dissipation

 Ongoing efforts to sensitize dissipation to mean-flow/turbulence length scales



Model fragmentation – dissipation components



• Component ε_{22}



Quasi-linear approximation

$$\Phi_{ij} = -C_1 \frac{\varepsilon}{k} \left(u_i u_j - \frac{2}{3} \delta_{ij} k \right) - C_2 \left(P_{ij} - \frac{2}{3} \delta_{ij} P_k \right) \quad (+\text{wall-reflection terms})$$

 Coefficients sensitized to anisotropy invariants, in compensation to the omission of high-order fragments

$$C_{1} = C + \sqrt{AE} \qquad C = 2.5A[\min\{0.6, A_{2}\}]^{1/4} f$$
$$f = \min\left\{ \left(\frac{\text{Re}_{t}}{150}\right)^{3/2}, 1 \right\}$$
$$C_{2} = 0.8A^{1/2}$$

Model fragmentation – pressure-velocity

• Sensitivity of coefficients to pressure-velocity interaction of \overline{uu}



Shock-induced Separation on 3D Jet-Afterbody - RSTM

• General view and surface-pressure coefficient



Shock-induced Separation on flat plate – LES

- Touber and Sandham, 2010
- *Re*₇=3000, M=2.3
- 20 M nodes, 240,000 CPU hours



- Fundamentally, Second-moment closure is far superior to eddyviscosity modelling.
- In reality, closure is extremely challenging, because the anisotropy is an extremely influential model element and is difficult to approximate.
- Redistribution and dissipation are especially influential.
- Many ways of construction models, but all involve calibration.
- Does involve "curve-fitting", but is based on rational principles and physically tenable assumptions.
- Little used, because of "the-simpler-the-better" attitude.
- Second-moment closure is inappropriately complex in (most) thin shear flows, but the only fundamentally solid approach in complex strain.