Subgrid-scale model based on the invariants of the gradient model tensor

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Overall perspective

- Direct Numerical Simulation: too many relevant scales of motion for practical cases
- Large eddy simulation. Models (Smagorinsky, Vreman, WALE...)
- Testing on benchmark cases (HIT, channel flow, boundary layer, driven cavity, sink flow...)

Our goal: combination of a pseudo-spectral method with the S3PQR algorithm. Testing on homogeneous isotropic turbulence (done), channel flow (done) and free boundary layer flow (work in progress)

Eddy viscosity - residual stress tensor

Incompressible Navier-Stokes equations:

$$\partial_t \overline{\boldsymbol{u}} + C(\overline{\boldsymbol{u}}, \overline{\boldsymbol{u}}) = D(\overline{\boldsymbol{u}}) - \nabla p - \nabla \tau(\overline{\boldsymbol{u}});$$
$$\nabla \cdot \overline{\boldsymbol{u}} = 0$$

- Eddy-viscosity closure model $\tau(\overline{\boldsymbol{u}}) \approx -2\nu_e S(\overline{\boldsymbol{u}})$ where $S(\overline{\boldsymbol{u}}) = 1/2(\nabla\overline{\boldsymbol{u}} + \nabla\overline{\boldsymbol{u}}^T)$ is the rate-of-strain tensor.
- $\nu_e = (C_m\Delta)^2 D_m(\overline{\boldsymbol{u}})$ where C_m is the model constant, Δ is the subgrid characteristic length, and $D_m(\overline{\boldsymbol{u}})$ is the differential operator with units of frequency associated with the model

Invariants of the gradient tensor

- From the several invariants of the gradient tensor $\mathsf{G} = \nabla \overline{\boldsymbol{u}}$, we restrict ourselves on

$$\{Q_{\mathsf{G}}, R_{\mathsf{G}}, Q_{\mathsf{S}}, R_{\mathsf{S}}, V_{\mathsf{G}}^2\}$$

where, given a second-order tensor A, we define

$$Q_A = (1/2)(tr^2(A) - tr(A^2))$$
$$R_A = det(A)$$
$$V_{\mathsf{G}}^2 = 4(tr(S^2\Omega^2) - 2Q_S Q_\Omega)$$
$$P_A = tr(A)$$

and $\mathsf{S} = 1/2(\mathsf{G} + \mathsf{G}^T)$ and $\Omega = 1/2(\mathsf{G} - \mathsf{G}^T)$ are the symmetric and the skew-symmetric parts of the gradient tensor, respectively.

Invariants of the gradient tensor

Most of the LES known models are based upon a combination of these invariants and can be written explicitly depending on them

- Smagorinsky model $\nu_e^{Smag} = f(Q_S)$
- Verstappen's model $\nu_e^{Ve} = f(R_S, Q_S)$
- WALE model $\nu_e^{W} = f(Q_G, V, Q_S)$
- Vreman's model $\nu_e^{Vr} = f(V, Q_G, Q_\Omega, Q_S)$
- σ-model $\nu_e^{\sigma} = f(GG^T eigenvalues)$

Invariants of the gradient tensor

- S3PQR models: involve three invariants of the symmetric tensor GG^T formally based on the lowest-order approximation of the subgrid stress tensor, $\tau(\overline{\boldsymbol{u}}) = \frac{\Delta^2}{12} GG^T + \mathcal{O}(\Delta^4)$
- These invariants are related with the original ones

$$P_{GG^T} = tr(GG^T) = 2(Q_\Omega - Q_S)$$
$$Q_{GG^T} = 2(Q_\Omega - Q_S)^2 - Q_G^2 + 4tr(S^2\Omega^2)$$
$$R_{GG^T} = det(GG^T) = det(G)det(G^T) = R_G^2$$

New models. S3PQR

We can construct new models of the form

$$\nu_e = (C_{s3pqr}\Delta)^2 P^p_{\mathrm{GG}^T} Q^q_{\mathrm{GG}^T} R^r_{\mathrm{GG}^T}$$

Restricting ourselves to solutions involving only two invariants of GG^T, three models are found

$$\nu_e^{S3PQ} = (C_{s3pq}\Delta)^2 P^{-5/2}_{\mathrm{GG}^T} Q^{3/2}_{\mathrm{GG}^T}$$

$$\nu_e^{S3PR} = (C_{s3pr}\Delta)^2 P^{-1}_{\mathrm{GG}^T} R^{1/2}_{\mathrm{GG}^T}$$

$$\nu_e^{S3QR} = (C_{s3qr}\Delta)^2 Q^{-1}_{\mathrm{GG}^T} R^{5/6}_{\mathrm{GG}^T}$$

S3PQR properties

Model constants

1. $C_{s3pq} = C_{s3pr} = C_{s3qr} = \sqrt{3} C_{Vr} \approx 0.458$ Numerical stability and less or equal dissipation than Vreman's model
2. $C_{s3pq} = 0.572$, $C_{s3pr} = 0.709$, $C_{s3qr} = 0.762$ The averaged dissipation of the models is equal than that of the Smagorinsky model. Simulations of decaying isotropic turbulence have shown that these values provides the right SGS dissipation.

2D Behaviour

- Only R_{GG^T}-dependent models switch off for 2D flows so S3PR and S3QR models are preferable

Other

- Positiveness, locality, Galilean invariance, proper near-wall behaviour

Generalities of the pseudo-spectral algorithm

- Pseudo-spectral method
- 3/2 rule de-aliasing technique
- Structured non-staggered grids
- Strong formulation. Poisson equation
- Fully-explicit second-order time-integration method
- MPI parallelization

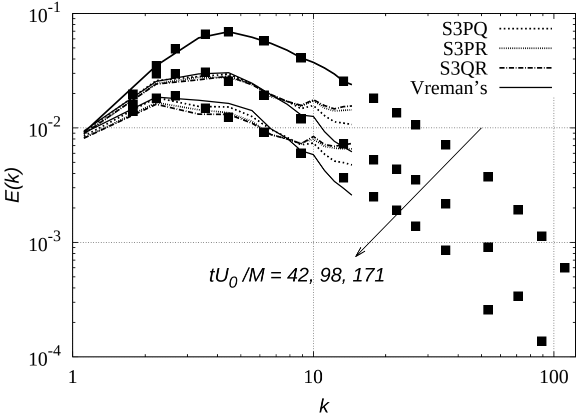
Successfully solved cases

- Homogeneous isotropic turbulence. Decaying and forced cases
- Channel flow

Test cases

Decaying isotropic turbulence with $C_{s3pq} = C_{s3pr} = C_{s3qr} = \sqrt{3}C_{Vr}$

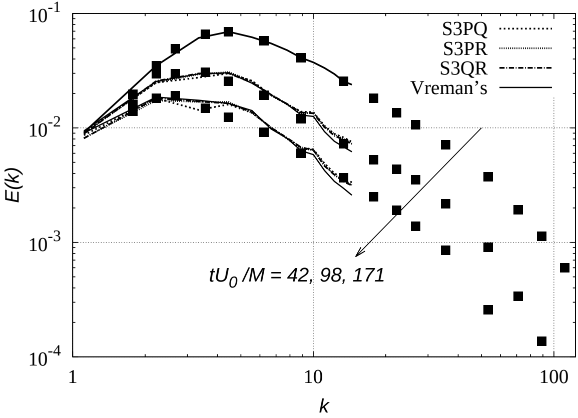
Comparison with classical Comte-Bellot & Corrsin (CBC) experiment.



Test cases

Decaying isotropic turbulence with $C_{s3pq} = 0.572,\ C_{s3pr} = 0.709,\ C_{s3qr} = 0.762$

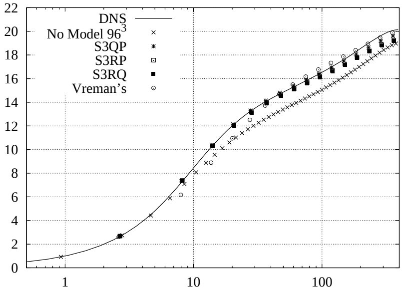
Comparison with classical Comte-Bellot & Corrsin (CBC) experiment.



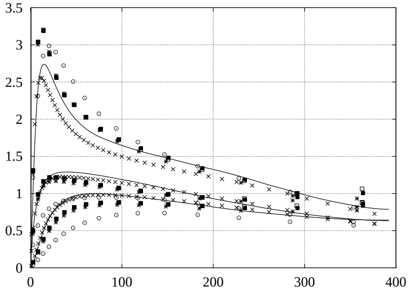
Test cases

Turbulent channel flow

$Re_\tau = 395$ DNS Moser et al. LES 32^3



mean velocity



rms fluctuations

Free boundary layer algorithm: current status

1. Currently developing and testing the algorithm
2. Pseudo-spectral methods demand periodic conditions: we follow Spalart's 1987[1],1988[2], that includes normal coordinate similarity transformations, growing terms and several other assumptions
3. Pseudo-spectral methods yield the maximum resolution when working with derivatives

[1] Spalart P.R., Leonard A. (1987) Direct Numerical Simulation of Equilibrium Turbulent Boundary Layers. https://doi.org/10.1007/978-3-642-71435-1_20

[2] Spalart, P. (1988). Direct simulation of a turbulent boundary layer up to $R_\theta = 1410$. doi:10.1017/S0022112088000345

Free boundary layer algorithm: current status

4. One of the issues of the boundary layer simulations is the semi infinite domain and the scaling procedure (sc).
   From $y\epsilon[0,\infty)$ to $y\epsilon[-1,1]$

Which is the performance of S3PQR algorithm under such conditions?

Free boundary layer: equation

$$\partial_t \overline{\boldsymbol{u}} + C_{sc}(\overline{\boldsymbol{u}}, \overline{\boldsymbol{u}}) + GT(\overline{\boldsymbol{u}}, \overline{U}) = D_{sc}\overline{\boldsymbol{u}} - \nabla_{sc} p - \nabla_{sc}\tau(\overline{\boldsymbol{u}});$$
$$\nabla_{sc} \cdot \overline{\boldsymbol{u}} = 0$$

- The most significant of these "growth terms" $GT(\overline{\boldsymbol{u}}, \overline{U})$ is the mean term, $(\overline{UU_X} + V\overline{U_\eta})$, in the x-momentum equation.This term supplies momentum to the boundary layer and allows it to maintain a statistically steady state, in spite of the momentum loss due to the shear stress at the wall[3]
- For simplicity, at this current approach we only consider $\overline{UU_X}$

[3] Spalart P.R., Leonard A. (1987) Direct Numerical Simulation of Equilibrium Turbulent Boundary Layers. https://doi.org/10.1007/978-3-642-71435-1_20

Free boundary layer: algorithm

- Direct adaptation of channel flow method
- Strong formulation. Poisson - pressure correction term. Chebyshev polynomials. Algebraic scaling.
- Explicit second order Adams - Bashforth scheme
- Boundary conditions

$$y = 0 \rightarrow u, v, w = 0$$

$$y = \infty \rightarrow < u >= 1; v, w = 0$$

- Zero mean pressure gradient

Boundary layer: scaling details

1. Algebraic scaling

$$y_\infty = L\frac{1+y_1}{1-y_1} \qquad \text{smooth } [0,\infty)$$

$$sc \equiv \frac{dy_1}{dy_\infty} \qquad \text{smooth } [2/L,0]$$

2. Convective term

$$u\frac{\partial u}{\partial x} + v\,sc\frac{\partial u}{\partial y_1} + w\frac{\partial u}{\partial z}$$

3. Diffusive term

$$\nu\left(\frac{\partial^2 u}{\partial x^2} + sc\frac{\partial}{\partial y_1}\left(sc\frac{\partial u}{\partial y_1}\right) + \frac{\partial^2 u}{\partial z^2}\right)$$

Boundary layer: scaling details

4 Poisson equation

$$\frac{\partial^2 P}{\partial x^2} + sc\frac{\partial}{\partial y_1}(sc\frac{\partial P}{\partial y_1}) + \frac{\partial^2 P}{\partial z^2} = \frac{\partial u}{\partial x} + sc\frac{\partial v}{\partial y_1} + \frac{\partial w}{\partial z}$$

5 S3PQR model

$$\frac{\partial}{\partial x}(\nu_e[\mathbf{x}]\frac{\partial u}{\partial x}) + sc\frac{\partial}{\partial y_1}(\nu_e[\mathbf{x}]sc\frac{\partial u}{\partial y_1}) + \frac{\partial}{\partial z}(\nu_e[\mathbf{x}]\frac{\partial u}{\partial z})$$

Scaling factor enters into the ν_e calculation via the Δ subgrid characteristic length and the invariants

Thank you for your attention.
Any questions?

Further reading

- F. X. Trias, D. Folch, A. Gorobets, and A. Oliva. Building proper invariants for eddy-viscosity subgrid-scale models. Physics of Fluids, 27(6):065103, 2015.
- R. A. Clark, J. H. Ferziger, and W. C. Reynolds. Evaluation of subgrid-scale models using an accurately simulated turbulent flow. Journal Fluid Mechanics, 91:1–16, 1979.
- F. X. Trias, D. Folch, A. Gorobets, and A. Oliva. Spectrally-consistent regularization of NavierStokes equations. Journal of Scientific Computing, 79:992–1014, 2019.