Building proper invariants for subgrid-scale eddy-viscosity models

F. Xavier Trias*, David Folch*, Andrey Gorobets*,*, Assensi Oliva*

*Heat and Mass Transfer Technological Center, Technical University of Catalonia
*Keldysh Institute of Applied Mathematics of RAS, Russia

15th European Turbulence Conference 2015
Delft (The Netherlands) August 25-28 2015
Contents

1. DNS of turbulence
2. Building proper invariants
3. New eddy-viscosity models
4. Results for a channel flow
5. Conclusions
DNS of turbulent incompressible flows

Main features of the DNS code:

- Structured staggered grids
- High-order symmetry-preserving schemes
- Fully-explicit second-order time-integration method
- Poisson solver for 2.5D problems: FFT + PCG
- Hybrid MPI+OpenMP parallelization
- OpenCL-based extension for its use on GPGPU

Air-filled differentially heated cavity at $Ra = 10^{11}$ (111M grid points), 2008

Plane impingement jet at $Re = 20000$ (102M grid points), 2011
DNS of turbulent incompressible flows

Square duct at $Re_\tau = 1200$ (172M grid points), 2013

Air-filled differentially heated cavity at $Ra = 10^{11}$ (111M grid points), 2008

Square cylinder at $Re = 22000$ (324M grid points), 2014

Plane impingement jet at $Re = 20000$ (102M grid points), 2011
DNS of turbulent incompressible flows

Square duct at $Re_\tau = 1200$ (172M grid points), 2013

Square cylinder at $Re = 22000$ (324M grid points), 2014

Rayleigh-Bénard convection at $Ra = 10^{10}$ (607M grid points), 2015
Scaling is possible\(^1\) … but never enough

Building proper invariants for LES models

Many turbulence **eddy-viscosity models** for LES have been proposed

\[
\partial_t \bar{u} + \mathcal{C}(\bar{u}, \bar{u}) = \mathcal{D}\bar{u} - \nabla \bar{p} - \nabla \cdot \tau(\bar{u}) \; ; \; \nabla \cdot \bar{u} = 0
\]

\[
\tau(\bar{u}) = -2\nu_t S(\bar{u})
\]
Many turbulence **eddy-viscosity models** for LES have been proposed

\[
\partial_t \bar{u} + C(\bar{u}, \bar{u}) = D\bar{u} - \nabla \bar{p} - \nabla \cdot \tau(\bar{u}) ; \quad \nabla \cdot \bar{u} = 0
\]

\[
\tau(\bar{u}) = -2\nu_t S(\bar{u})
\]

... most of them **rely on differential operators** that are **based on the combination of invariants** of a symmetric second-order tensor derived from \( G \equiv \nabla \bar{u} \).
Many turbulence **eddy-viscosity models** for LES have been proposed

\[
\partial_t \bar{u} + C(\bar{u}, \bar{u}) = D\bar{u} - \nabla p - \nabla \cdot \tau(\bar{u}) \quad ; \quad \nabla \cdot \bar{u} = 0
\]

\[
\tau(\bar{u}) = -2\nu_t S(\bar{u})
\]

... most of them **rely on differential operators** that are **based on the combination of invariants** of a symmetric second-order tensor derived from \( G \equiv \nabla \bar{u} \).

Therefore, they can be characterized by 5 **basic invariants**

\[
\{ Q_S, R_S, Q_G, R_G, V^2 \}
\]
Many turbulence **eddy-viscosity models** for LES have been proposed

\[
\partial_t \bar{u} + C(\bar{u}, \bar{u}) = \mathcal{D} \bar{u} - \nabla \bar{p} - \nabla \cdot \tau(\bar{u}) ; \quad \nabla \cdot \bar{u} = 0
\]

\[
\tau(\bar{u}) = -2\nu_t S(\bar{u})
\]

... most of them **rely on differential operators** that are based on the combination of **invariants** of a symmetric second-order tensor derived from \( G \equiv \nabla \bar{u} \).

Therefore, they can be characterized by 5 **basic invariants**

\[
\{ Q_S, R_S, Q_G, R_G, V^2 \}
\]

**Notation**: given a second-order tensor \( A \)

First invariant: \( P_A = tr(A) \)

Second invariant: \( Q_A = 1/2\{tr^2(A) - tr(A^2)\} \)

Third invariant: \( R_A = det(A) \)
Building proper invariants for LES models

Many turbulence **eddy-viscosity models** for LES have been proposed

\[ \partial_t \overline{u} + \mathcal{C}(\overline{u}, \overline{u}) = D\overline{u} - \nabla \overline{p} - \nabla \cdot \tau(\overline{u}) ; \quad \nabla \cdot \overline{u} = 0 \]

\[ \tau(\overline{u}) = -2\nu_t S(\overline{u}) \]

... most of them rely on differential operators that are based on the combination of invariants of a symmetric second-order tensor derived from \( G \equiv \nabla \overline{u} \).

Therefore, they can be characterized by 5 **basic invariants**

\[ \{ Q_S, R_S, Q_G, R_G, V^2 \} \]

**Notation:**

\[ V^2 = 4(\text{tr}(S^2\Omega^2) - 2Q SQ\Omega), \]

where \( S = 1/2(G + G^T) \) and \( \Omega = 1/2(G - G^T) \).
A unified framework for eddy-viscosity models

\{ Q_S, R_S, Q_G, R_G, V^2 \}
A unified framework for eddy-viscosity models

\{ Q_S, R_S, Q_G, R_G, V^2 \}

Smagorinsky model

\[ \nu_{e,\text{Smag}} = (C_S \Delta)^2 |S(\bar{u})| = 2(C_S \delta)^2 (-Q_S)^{1/2}, \]
A unified framework for eddy-viscosity models

\{Q_S, R_S, Q_G, R_G, V^2\}

Smagorinsky model
\[ \nu_e^{Smag} = (C_S \Delta)^2 |S(\bar{u})| = 2(C_S \delta)^2 (-Q_S)^{1/2}, \]

Verstappen’s model
\[ \nu_e^{Ve} = (C_{Ve} \Delta)^2 \frac{|R_S|}{-Q_S}, \]
A unified framework for eddy-viscosity models

\[ \{ Q_S, R_S, Q_G, R_G, V^2 \} \]

Smagorinsky model

\[ \nu_{e}^{Smag} = (C_S \Delta)^2 |S(\bar{u})| = 2(C_S \delta)^2 (-Q_S)^{1/2}, \]

Verstappen’s model

\[ \nu_{e}^{Ve} = (C_{Ve} \Delta)^2 \frac{|R_S|}{-Q_S}, \]

WALE model

\[ \nu_{e}^{W} = (C_{W} \Delta)^2 \frac{(V^2/2 + 2Q_G^2/3)^{3/2}}{(-2Q_S)^{5/2} + (V^2/2 + 2Q_G^2/3)^{5/4}}, \]

where \( \sigma_i = \sqrt{\lambda_i} \) and \( \lambda_i \) is an eigenvalue of \( GG^T \).
A unified framework for eddy-viscosity models

\{ Q_S, R_S, Q_G, R_G, V^2 \}

Smagorinsky model
\[ \nu^\text{Smag}_e = (C_S \Delta)^2 |S(\overline{u})| = 2(C_S \delta)^2 (-Q_S)^{1/2}, \]

Verstappen’s model
\[ \nu^\text{Ve}_e = (C_{Ve} \Delta)^2 \frac{|R_S|}{-Q_S}, \]

WALE model
\[ \nu^\text{W}_e = (C_W \Delta)^2 \frac{(V^2/2 + 2Q_G^2/3)^{3/2}}{(-2Q_S)^{5/2} + (V^2/2 + 2Q_G^2/3)^{5/4}}, \]

Vreman’s model
\[ \nu^\text{Vr}_e = (C_{Vr} \Delta)^2 \left( \frac{V^2 + Q_G^2}{2(Q_\Omega - Q_S)} \right)^{1/2}, \]
A unified framework for eddy-viscosity models

\[
\{ Q_S, R_S, Q_G, R_G, V^2 \}
\]

Smagorinsky model
\[
\nu_e^{Smag} = (C_S \Delta)^2 |S(\bar{u})| = 2(C_S \delta)^2 (-Q_S)^{1/2},
\]

Verstappen’s model
\[
\nu_e^{Ve} = (C_{Ve} \Delta)^2 \frac{|R_S|}{-Q_S},
\]

WALE model
\[
\nu_e^{W} = (C_W \Delta)^2 \frac{(V^2/2 + 2Q_G^2/3)^{3/2}}{(-2Q_S)^{5/2} + (V^2/2 + 2Q_G^2/3)^{5/4}},
\]

Vreman’s model
\[
\nu_e^{Vr} = (C_{Vr} \Delta)^2 \left( \frac{V^2 + Q_G^2}{2(Q_\Omega - Q_S)} \right)^{1/2},
\]

Sigma model
\[
\nu_e^{\sigma} = (C_{\sigma} \Delta)^2 \frac{\sigma_3(\sigma_1 - \sigma_2)(\sigma_2 - \sigma_3)}{\sigma_1^2},
\]

where \( \sigma_i = \sqrt{\lambda_i} \) and \( \lambda_i \) is an eigenvalue of \( GG^T \).
Near-wall behavior

\{ Q_s, R_S, Q_G, R_G, V^2 \}
Near-wall behavior

\[
\{Q_S, R_S, Q_G, R_G, V^2\}
\]

<table>
<thead>
<tr>
<th>Wall-behavior</th>
<th>Invariants</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q_G</td>
<td>R_G</td>
</tr>
<tr>
<td>Units</td>
<td>O(y^2)</td>
</tr>
<tr>
<td></td>
<td>[T^{-2}]</td>
</tr>
</tbody>
</table>
Near-wall behavior

\[ \{ Q_S, R_S, Q_G, R_G, V^2 \} \]

<table>
<thead>
<tr>
<th>Wall-behavior</th>
<th>Invariants</th>
<th>Units</th>
<th>Models</th>
</tr>
</thead>
<tbody>
<tr>
<td>Units</td>
<td>( Q_G )</td>
<td>( O(y^2) )</td>
<td>( O(y^3) )</td>
</tr>
<tr>
<td>[T^{-2}]</td>
<td>[T^{-3}]</td>
<td>[T^{-2}]</td>
<td>[T^{-3}]</td>
</tr>
<tr>
<td>Wall-behavior</td>
<td>( R_G )</td>
<td>( O(y^0) )</td>
<td>( O(y^1) )</td>
</tr>
<tr>
<td>Smagorinsky</td>
<td>( Q_S )</td>
<td>( O(y^0) )</td>
<td>( O(y^1) )</td>
</tr>
<tr>
<td>WALE</td>
<td>( R_S )</td>
<td>( O(y^0) )</td>
<td>( O(y^1) )</td>
</tr>
<tr>
<td>Vreman's</td>
<td>( V^2 )</td>
<td>( O(y^0) )</td>
<td>( O(y^1) )</td>
</tr>
<tr>
<td>Verstappen's</td>
<td>( Q_\Omega )</td>
<td>( O(y^0) )</td>
<td>( O(y^1) )</td>
</tr>
<tr>
<td>( \sigma )-model</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Hence, new models can be derived by imposing restrictions on the differential operators they are based on.
Near-wall behavior

\[ \{ Q_S, R_S, Q_G, R_G, V^2 \} \]

<table>
<thead>
<tr>
<th>Wall-behavior</th>
<th>Invariants</th>
<th>Models</th>
</tr>
</thead>
<tbody>
<tr>
<td>Units</td>
<td>( Q_G )</td>
<td>Smagorinsky</td>
</tr>
<tr>
<td></td>
<td>( R_G )</td>
<td>WALE</td>
</tr>
<tr>
<td></td>
<td>( Q_S )</td>
<td>Vreman's</td>
</tr>
<tr>
<td></td>
<td>( R_S )</td>
<td>Verstappen's</td>
</tr>
<tr>
<td></td>
<td>( V^2 )</td>
<td>( \sigma )-model</td>
</tr>
<tr>
<td></td>
<td>( Q_\Omega )</td>
<td></td>
</tr>
</tbody>
</table>

Hence, new models can be derived by imposing restrictions on the differential operators they are based on.
For instance, let us consider models that are based on the invariants of the tensor $GG^T$

$$\nu_e = (C_M \delta)^2 P_{GG^T}^p Q_{GG^T}^q R_{GG^T}^r,$$

---

Building proper invariants for LES models

For instance, let us consider models that are based on the invariants of the tensor $G G^T$

$$\nu_e = (C_M \delta)^2 P_{GG^T}^p Q_{GG^T}^q R_{GG^T}^r,$$

<table>
<thead>
<tr>
<th>Formula</th>
<th>$2(Q_{\Omega} - Q_S)$</th>
<th>$V^2 + Q_G^2$</th>
<th>$R_G^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{GG^T}$</td>
<td>$Q_{GG^T}$</td>
<td>$R_{GG^T}$</td>
<td></td>
</tr>
</tbody>
</table>

---

Building proper invariants for LES models\textsuperscript{2}

For instance, let us consider models that are based on the invariants of the tensor $GG^T$

$$\nu_e = (C_M \delta)^2 P_{GG^T}^p Q_{GG^T}^q R_{GG^T}^r,$$

<table>
<thead>
<tr>
<th></th>
<th>$P_{GG^T}$</th>
<th>$Q_{GG^T}$</th>
<th>$R_{GG^T}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula</td>
<td>$2(Q_\Omega - Q_S)$</td>
<td>$V^2 + Q_G^2$</td>
<td>$R_G^2$</td>
</tr>
<tr>
<td>Wall-behavior</td>
<td>$O(y^0)$</td>
<td>$O(y^2)$</td>
<td>$O(y^6)$</td>
</tr>
<tr>
<td>Units</td>
<td>$[T^{-2}]$</td>
<td>$[T^{-4}]$</td>
<td>$[T^{-6}]$</td>
</tr>
</tbody>
</table>

Building proper invariants for LES models

For instance, let us consider models that are based on the invariants of the tensor $GG^T$

$$\nu_e = (C_M \delta)^2 P_{GG^T}^{P} Q_{GG^T}^{q} R_{GG^T}^{r},$$

<table>
<thead>
<tr>
<th></th>
<th>$P_{GG^T}$</th>
<th>$Q_{GG^T}$</th>
<th>$R_{GG^T}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula</td>
<td>$2(Q_{\Omega} - Q_S)$</td>
<td>$V^2 + Q_G^2$</td>
<td>$R_G^2$</td>
</tr>
<tr>
<td>Wall-behavior</td>
<td>$O(y^0)$</td>
<td>$O(y^2)$</td>
<td>$O(y^6)$</td>
</tr>
<tr>
<td>Units</td>
<td>$[T^{-2}]$</td>
<td>$[T^{-4}]$</td>
<td>$[T^{-6}]$</td>
</tr>
</tbody>
</table>

$$-6r - 4q - 2p = -1; \quad 6r + 2q = s,$$

where $s$ is the slope for the asymptotic near-wall behavior, i.e. $O(y^s)$.

---

Building proper invariants for LES models

Solutions: \( q(p, s) = (1 - s)/2 - p \) and \( r(p, s) = (2s - 1)/6 + p/3 \)
Building proper invariants for LES models

Solutions: \( q(p, s) = (1 - s)/2 - p \) and \( r(p, s) = (2s - 1)/6 + p/3 \)

![Graph showing the functions q(p) and r(p)]
Building proper invariants for LES models

Solutions: \( q(p, s) = (1 - s)/2 - p \) and \( r(p, s) = (2s - 1)/6 + p/3 \)
Building proper invariants for LES models

Solutions: \( q(p, s) = (1 - s)/2 - p \) and \( r(p, s) = (2s - 1)/6 + p/3 \)
Building proper models for LES

Hence, a family of **new eddy-viscosity** model for LES

\[
\partial_t \bar{u} + C(\bar{u}, \bar{u}) = D \bar{u} - \nabla p - \nabla \cdot \tau(\bar{u}) ; \quad \nabla \cdot \bar{u} = 0
\]

\[
\tau(\bar{u}) = -2\nu_e S(\bar{u})
\]
Hence, a family of **new eddy-viscosity** model for LES

\[
\partial_t \overline{u} + C(\overline{u}, \overline{u}) = \mathcal{D} \overline{u} - \nabla \overline{p} - \nabla \cdot \tau(\overline{u}) ; \quad \nabla \cdot \overline{u} = 0
\]

\[
\tau(\overline{u}) = -2\nu_e S(\overline{u})
\]

has been derived by **imposing proper conditions** on the invariant(s)

\[
\nu_{eS3QP} = (C_{s3qp}\delta)^2 P_{GGT}^{-5/2} Q_{GGT}^{3/2},
\]

\[
\nu_{eS3RP} = (C_{s3rp}\delta)^2 P_{GGT}^{-1} R_{GGT}^{1/2},
\]

\[
\nu_{eS3RQ} = (C_{s3rq}\delta)^2 Q_{GGT}^{-1} R_{GGT}^{5/6}.
\]
Building proper models for LES

Hence, a family of **new eddy-viscosity** model for LES

\[
\partial_t \bar{u} + C(\bar{u}, \bar{u}) = D\bar{u} - \nabla\bar{p} - \nabla \cdot \tau(\bar{u}); \quad \nabla \cdot \bar{u} = 0
\]

\[
\tau(\bar{u}) = -2\nu_e S(\bar{u})
\]

has been derived by **imposing proper conditions** on the invariant(s)

\[
\nu_e^{S3QP} = (C_{s3qp}\delta)^2 P^{-5/2}_{GG_T} Q^{3/2}_{GG_T},
\]

\[
\nu_e^{S3RP} = (C_{s3rp}\delta)^2 P^{-1}_{GG_T} R^{1/2}_{GG_T},
\]

\[
\nu_e^{S3RQ} = (C_{s3rq}\delta)^2 Q^{-1}_{GG_T} R^{5/6}_{GG_T}.
\]

And what about the model **constants**?
Building proper models for LES

Finding model constants

The model constants, $C_{s3xx}$, can be related with the Vreman’s constant, $C_{Vr}$, with the following inequality

$$0 \leq \frac{(C_{Vr})^2 \nu e^{S3xx}}{(C_{s3xx})^2 \nu e^{Vr}} \leq \frac{1}{3}.$$
The model constants, $C_{s3xx}$, can be related with the Vreman’s constant, $C_{Vr}$, with the following inequality

$$0 \leq \frac{(C_{Vr})^2 \nu_e^{s3xx}}{(C_{s3xx})^2 \nu_e^{Vr}} \leq \frac{1}{3}.$$ 

Hence, imposing that $C_{s3qp} = C_{s3rp} = C_{s3rq} = \sqrt{3}C_{Vr}$ guarantees:

$$\nu_e^{s3xx}$$
The model constants, $C_{s3xx}$, can be related with the Vreman’s constant, $C_{Vr}$, with the following inequality

$$0 \leq \frac{(C_{Vr})^2}{(C_{s3xx})^2} \frac{\nu_e^{s3xx}}{\nu_{Ve}^{Vr}} \leq \frac{1}{3}.$$ 

Hence, imposing that $C_{s3qp} = C_{s3rp} = C_{s3rq} = \sqrt{3}C_{Vr}$ guarantees:

$$0 \leq \nu_e^{s3xx}$$

numerical stability
Building proper models for LES
Finding model constants

The model constants, \( C_{s3xx} \), can be related with the Vreman’s constant, \( C_{Vr} \), with the following inequality

\[
0 \leq \frac{(C_{Vr})^2}{(C_{s3xx})^2} \frac{\nu_{e}^{s3xx}}{\nu_{e}^{Vr}} \leq \frac{1}{3}.
\]

Hence, imposing that \( C_{s3qp} = C_{s3rp} = C_{s3rq} = \sqrt{3} C_{Vr} \) guarantees:

\[
0 \leq \nu_{e}^{s3xx} \leq \nu_{e}^{Vr}
\]

numerical stability less or equal dissipation than Vreman’s model!
Building proper models for LES

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

Comparison with classical Comte-Bellot & Corrsin (CBC) experiment.
Building proper models for LES
Decaying isotropic turbulence with $C_{s3pq} = 0.572$, $C_{s3pr} = 0.709$, $C_{s3qr} = 0.762$

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

Results

\[ Re_\tau = 395 \]

DNS Moser et al.

LES 32^3

mean velocity

rms fluctuations

Building proper invariants for subgrid-scale eddy-viscosity models
Turbulent channel flow
Near-wall behavior

32x32x32

32x96x32

Building proper invariants for subgrid-scale eddy-viscosity models
Most of the existing eddy-viscosity models for LES can be represented into this 5D phase space of invariants

\[ \{ Q_S, R_S, Q_G, R_G, V^2 \} \]
Conclusions

- Most of the existing eddy-viscosity models for LES can be represented into this 5D phase space of invariants

\[ \{ Q_S, R_S, Q_G, R_G, V^2 \} \]

- Based on this general framework, a family of new eddy-viscosity type LES models has been derived by imposing proper restrictions.
Conclusions

- Most of the existing eddy-viscosity models for LES can be represented into this 5D phase space of invariants

\[ \{ Q_S, R_S, Q_G, R_G, V^2 \} \]

- Based on this general framework, a family of **new eddy-viscosity type** LES models has been derived by imposing proper restrictions.
Conclusions and Future Research

- Most of the existing eddy-viscosity models for LES can be represented into this 5D phase space of invariants

\[ \{ Q_S, R_S, Q_G, R_G, V^2 \} \]

- Based on this general framework, a family of **new eddy-viscosity type** LES models has been derived by imposing proper restrictions.

- Test the performance of new eddy-viscosity type LES for different configurations.
Thank you for your attention
Building proper invariants for eddy-viscosity subgrid-scale models

F. X. Trias, 1,a) D. Folch, 1,b) A. Gorobets, 1,2,c) and A. Oliva 1,d)

1Heat and Mass Transfer Technological Center, Technical University of Catalonia, ETSEIAT,
c/Colom 11, 08222 Terrassa, Spain
2Keldysh Institute of Applied Mathematics, Miusskaya Sq. 4A, Moscow 125047, Russia

(Received 31 March 2015; accepted 16 May 2015; published online 2 June 2015)