New differential operators and discretization methods for large-eddy simulation and regularization modeling

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New differential operators and discretization methods for LES and regularization modeling
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)

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

Turbulent square duct at $Re_\tau = 1200$ (172M grid points)

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

Square cylinder at $Re = 22000$ (300M grid points)

Plane impingement jet at $Re = 20000$ (102M grid points)
Scaling is possible\(^1\)… but never enough

\[\text{Normalized speedup} = \frac{\text{Speedup}}{\text{Linear Speedup}}\]

\[\text{Number of CPU cores} = 1600, 3200, 6400, 12800\]

\[256 \times 800 \times 1600 \quad (327.7\text{M})\]

\[256 \times 1400 \times 2800 \quad (1003.5\text{M})\]

\[\text{70\% efficiency}\]

\(^1\)A. Gorobets et al. “Hybrid MPI+OpenMP parallelization of an FFT-based 3D Poisson solver with one periodic direction” Computers\&Fluids, 49:101-109, 2011
Governing equations

Incompressible Navier-Stokes equations:

\[ \nabla \cdot u = 0 \]
\[ \partial_t u + C(u, u) = D u - \nabla p \]

where the **nonlinear convective** term is given by

\[ C(u, \phi) = (u \cdot \nabla)\phi \]

and the **linear dissipative** term is given by

\[ D\phi = \nu \Delta \phi \]
When does a turbulence should switch on/off?

Taking the curl of momentum equation the \textit{vorticity transport equation} follows

\[
\partial_t \omega + C(u, \omega) = C(\omega, u) + D(\omega)
\]

Let us now consider an arbitrary part of the flow domain, \( \Omega \), with \textit{periodic boundary conditions}. Then, taking the \( L^2 \) innerproduct with \( \omega = \nabla \times u \) leads to the \textit{enstrophy equation}

\[
\frac{1}{2} \frac{d}{dt} (\omega, \omega) = (\omega, C(\omega, u)) - \nu (\nabla \omega, \nabla \omega)
\]

where \((a, b) = \int_\Omega a \cdot b d\Omega\). Unless, the grid is fine enough convection dominates diffusion (in a discrete sense)

\[
(\omega, C(\omega, u)) > \nu (\nabla \omega, \nabla \omega)
\]
When does a turbulence should switch on/off?

The vortex-stretching term can be expressed in terms of the invariant \( R_S = -1/3 \text{tr}(S^3) = -\text{det}(S) \)

\[
(\omega, C(\omega, u)) = 4 \int_\Omega R_S d\Omega
\]

whereas the \( L^2(\Omega) \)-norm of \( \omega \) in terms of the invariant \( Q_S = -1/2 \text{tr}(S^2) \)

\[
\nu(\nabla \omega, \nabla \omega) = \nu(\omega, \Delta \omega) \leq -\nu \lambda_\Delta(\omega, \omega) = 4\nu \lambda_\Delta \int_\Omega Q_S d\Omega
\]

where \( \lambda_\Delta < 0 \) is the largest (smallest in absolute value) non-zero eigenvalue of Laplacian operator \( \Delta \) on \( \Omega \). In a periodic box of size \( h \),

\[
\lambda_\Delta = -(\pi/h)^2.
\]
When does a turbulence should switch on/off?

Therefore, the **overall damping** introduced by a model should be given by

\[
H^\Omega = \min \left\{ \frac{\nu \lambda \Delta \tilde{Q}_S}{|\tilde{R}_S|}, 1 \right\}
\]

where \(\tilde{R}_S = \int_{\Omega} R_S d\Omega\) and \(\tilde{Q}_S = \int_{\Omega} Q_S d\Omega\).

Notice that any model based on this ratio automatically **switches off** for:

- Laminar flows \((R_S \rightarrow 0)\)
- 2D flows \((\lambda_2 = 0 \rightarrow R_S = 0)\)
- In the wall (near-wall behavior is given by \(R_S \propto y^1\) and \(Q_S \propto y^0\))
An eddy-viscosity model for LES

Therefore, the **overall damping** introduced by a model should be given by

\[
H^\Omega = \min \left\{ \frac{\nu \lambda_\Delta \tilde{Q}_S}{|\tilde{R}_S|}, 1 \right\}
\]

One possible solution would consist on an **eddy-viscosity** type LES model:

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

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

\[
\nu_t \approx \frac{|\tilde{R}_S|}{\lambda_\Delta \tilde{Q}_S}
\]

---

Results for a turbulent channel flow\(^2\)

\[ Re_\tau = 590 \]

DNS Moser et al.  
LES 64\(^3\)

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Mean velocity

Rms fluctuations

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New differential operators and discretization methods for LES and regularization modeling
Regularization modeling

Therefore, the **overall damping** introduced by a model should be given by

\[
H^\Omega = \min \left\{ \frac{\nu \lambda \Delta \tilde{Q}_S}{|\tilde{R}_S|}, 1 \right\}
\]

Alternatively, **regularizations** of the non-linear convective term results into a damping of vortex-stretching term, *i.e.* \( f^{\text{reg}} |\tilde{R}_S| \) (where \( 0 < f^{\text{ref}} \leq 1 \))

\[
f^{\text{reg}} \approx \min \left\{ \frac{\nu \lambda \Delta \tilde{Q}_S}{|\tilde{R}_S|}, 1 \right\}
\]

Or a combination of both?
Results for a differentially heated cavity at $Ra = 4.5 \times 10^{10}$

- Regularization model $C_4$ is tested.

\[
\partial_t u_\epsilon + C_4(u_\epsilon, u_\epsilon) = D(u_\epsilon) - \nabla p_\epsilon
\]

where the convective term is smoothed as

\[
C_4(u, v) = C(\bar{u}, \bar{v}) + C(\bar{u}, v') + C(u', \bar{v})
\]

- Two coarse meshes are considered

<table>
<thead>
<tr>
<th></th>
<th>DNS</th>
<th>RM1</th>
<th>RM2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_x$</td>
<td>128</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>$N_y$</td>
<td>318</td>
<td>12</td>
<td>14</td>
</tr>
<tr>
<td>$N_z$</td>
<td>862</td>
<td>54</td>
<td>38</td>
</tr>
</tbody>
</table>
Results for differentially heated cavity at $Ra = 4.5 \times 10^{10}$

Profiles

Averaged vertical velocity and temperature at the horizontal mid-height plane.

Challenging $C_4$: mesh independence analysis

The overall Nusselt number and the centerline stratification for 50 randomly generated coarse grids with fixed stretching at $Ra = 4.5 \times 10^{10}$.

$8 \leq N_x \leq 12$, $16 \leq N_y \leq 28$, and $44 \leq N_z \leq 70$. 

New differential operators and discretization methods for LES and regularization modeling
Building proper invariants for LES models

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

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

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

... most of them rely on differential operators that are based on the combination of invariants of a symmetric second-order tensor derived from \( G \equiv \nabla \bar{u} \). It can be characterized by 5 basic invariants

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

where \( Q_A = 1/2\{ tr^2(A) - tr(A^2) \} \) and \( R_A = det(A) \) represent the second and third invariants of the second-order tensor \( A \), respectively. Moreover, the first invariant of \( A \) will be denoted as \( P_A = tr(A) \).

\[
V^2 = tr(S^2 \Omega^2), \quad \text{where} \quad S = 1/2(G + G^T) \quad \text{and} \quad \Omega = 1/2(G - G^T).
\]
A unified framework for eddy-viscosity models

\[ R_S\text{-based model} \quad \nu_e^R = (C_R \delta)^2 \frac{|R_S|}{-Q_S}, \]

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

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

Vreman’s model \[ \nu_e^{Vr} = (C_{Vr} \delta)^2 \left( \frac{Q_G^2 + 4Z^2}{2(Q\Omega - Q_S)} \right)^{1/2}, \]

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

where \( \sigma_i \) are the three singular eigenvalues of \( G \), i.e. \( \sigma_i = \sqrt{\lambda_i} \) where \( \lambda_i \) is an eigenvalue of \( GG^T \), \( Z^2 = V^2 - 2Q_SQ_\Omega \) and \( Q_G = Q_S + Q_\Omega \).
Near-wall behavior

<table>
<thead>
<tr>
<th>Wall-behavior</th>
<th>Units</th>
<th>Invariants</th>
<th>Models</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$Q_G$</td>
<td>Smagorinsky</td>
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<tr>
<td></td>
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<td>$R_G$</td>
<td>WALE</td>
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<td>$Q_S$</td>
<td>Vreman’s</td>
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<td></td>
<td></td>
<td>$R_S$</td>
<td>$R_S$-based</td>
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<tr>
<td></td>
<td></td>
<td>$V^2$</td>
<td>$\sigma$-model</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$Q_\Omega$</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$Z^2$</td>
<td></td>
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</tbody>
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Hence, new models can be derived by imposing restrictions on the differential operators they are based on.
Building proper invariants for LES models

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

$$\nu_e = (C_M \delta)^2 P^{p}_{GG^T} Q^{q}_{GG^T} R^{r}_{GG^T},$$

<table>
<thead>
<tr>
<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>$Q_{G}^2 + 4Z^2$</td>
</tr>
<tr>
<td>Wall-behavior</td>
<td>$\mathcal{O}(y^0)$</td>
<td>$\mathcal{O}(y^2)$</td>
</tr>
<tr>
<td>Units</td>
<td>$[T^{-2}]$</td>
<td>$[T^{-4}]$</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. $\mathcal{O}(y^s)$. 
Building proper invariants for LES models

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

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

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

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

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

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

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

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

And what about the implementation?

- Given \( G \equiv \nabla \bar{u} \ldots \) no problem to compute \( P_{GG_T}, Q_{GG_T}, R_{GG_T} \)
- But, what about the **discretization** of \( \nabla \cdot \tau(\bar{u}) \) ?

New differential operators and discretization methods for LES and regularization modeling
Discretization of $2\nabla \cdot (\nu_t S(u))$: a new simple approach\textsuperscript{4}

\[
\partial_t u + C(u, u) = Du - \nabla p + 2\nabla \cdot (\nu_t S(u)), \quad \nabla \cdot u = 0
\]
\[
\Omega_s \frac{du_s}{dt} + C(u_s)u_s = Du_s + M^T p_c + \text{??????}, \quad M u_s = 0_c
\]

where $2\nabla \cdot (\nu_t S(u)) = \nabla \cdot (\nu_t \nabla u) + \nabla \cdot (\nu_t \nabla u^T)$.\[
\nabla \cdot (\nu_t \nabla u^T) = \nabla (\nabla \cdot (\nu_t u)) - \nabla \cdot (u \otimes \nabla \nu_t)
\]
\[
= \nabla (\nabla \cdot (\nu_t u)) - C(u, \nabla \nu_t)
\]

where $[\tilde{u}_s]_f = [\nu_t, s]_f[u_s]_f$. \textit{Straightforward implementation}!!!

\textsuperscript{4}F.X. Trias \textit{et al.} \textit{A simple approach to discretize the viscous term with spatially varying (eddy-)viscosity} \textit{Journal of Computational Physics}, 253:405-417, 2013
Discretization of $2\nabla \cdot (\nu_t S(u))$: a new simple approach

$4^{th}$-order FVM on a staggered Cartesian grid
Discretization of $2\nabla \cdot \left( \nu_t S(u) \right)$: a new simple approach

$2^{th}$-order FVM on a collocated unstructured grid
Discretization of $2\nabla \cdot (\nu_t S(u))$: a new simple approach

Let’s make it even easier...

\[
\nabla \cdot (\nu_t \nabla u^T) = \nabla (\nabla \cdot (\nu_t u)) - C(u, \nabla \nu_t)
\]

\[
\begin{align*}
- \mathbf{M}^T \Omega_c^{-1} \mathbf{M} \tilde{u}_s - C(u_s)(-\Omega_s^{-1} \mathbf{M}^T \nu_{t,c}) \\
\approx \nabla (\nabla \cdot (\nu_t u)) - C(u, \nabla \nu_t)
\end{align*}
\]

Since $\nabla (\nabla \cdot (\nu_t u))$ is a gradient of a scalar field, this term can be absorbed into the pressure, $\pi = p - \nabla \cdot (\nu_t u)$.

Therefore, the only term that needs to be discretized is

\[
\begin{align*}
- C(u_s)(-\Omega_s^{-1} \mathbf{M}^T \nu_{t,c}) \\
\approx C(u, \nabla \nu_t)
\end{align*}
\]
Conclusions and Future Research

- Most of the existing eddy-viscosity (also regularization) 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.

- A simple **new approach to discretize** the viscous term for **eddy-viscosity models** has been proposed.

- Test the performance of new eddy-viscosity type LES for different configurations.

- Try to properly combine **regularization modeling** and **LES**.
Thank you for your attention
Further reading

