New differential operators and discretization methods for eddy-viscosity models for LES

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Contents

1. DNS of turbulence
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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)

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

Wall-mounted cube at $Re = 7240$ (17M grid points)

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

Square cylinder at $Re = 22000$ (75M grid points)

Plane impingement jet at $Re = 20000$ (102M grid points)
New DNS: turbulent square duct up to at $Re_\tau = 1200$

Some details about DNS at $Re_\tau = 1200$

- Mesh size: $640 \times 518 \times 518$
- 392 CPUs on the MareNostrum ($P_x = 2$, $P_y = 14$, $P_z = 14$)
- $4^{th}$-order symmetry-preserving scheme
- $Re_\tau = 1200$
New DNS: turbulent square duct up to at $Re_{τ} = 1200$

Some details about **DNS** at $Re_{τ} = 1200$

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- $Re_{τ} = 1200$
Scaling? Yes\textsuperscript{1}, we can... but never enough

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{speedup_graph}
\caption{Normalized speedup as a function of the number of CPU cores for different problem sizes and configurations.}
\end{figure}

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

Incompressible Navier-Stokes equations:

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

\[ D\phi = \nu \Delta \phi \]
Stopping the vortex-stretching

Taking the curl of momentum equation the vorticity transport equation follows

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

\(^2\)F.X. Trias et al. Computers\&Fluids, 39:1815-1831, 2010
Stopping the vortex-stretching

Taking the curl of momentum equation the **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 periodic boundary conditions. Then, taking the $L^2$ innerproduct with $\omega = \nabla \times u$ leads to the **enstrophy equation**

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

where $(a, b) = \int_{\Omega} a \cdot b d\Omega$.

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

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

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\]

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

\[
(\omega, C(\omega, u)) > \nu (\nabla \omega, \nabla \omega)
\]

\footnote{F.X. Trias \textit{et al.} \textit{Computers\&Fluids}, 39:1815-1831, 2010}
Stopping the vortex-stretching

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

\[ (\omega, C(\omega, u)) = 4 \int_{\Omega} R d\Omega \]
Stopping the vortex-stretching

The vortex-stretching term can be expressed in terms of the invariant
\[ R = -\frac{1}{3} tr(S^3) = -\det(S) \]

Then, recalling that \( \nabla \times \omega = \nabla (\nabla \cdot u) - \Delta u \) and the boundary contribution vanishes *, the diffusive term is given by the \( L^2(\Omega) \)-norm of \( \Delta u \)

\[ (\nabla \omega, \nabla \omega) \overset{*}{=} - (\omega, \Delta \omega) = (\omega, \nabla \times \nabla \times \omega) \]

\[ \overset{*}{=} (\nabla \times \omega, \nabla \times \omega) = (\Delta u, \Delta u) = \| \Delta u \|^2 \]
The **overall damping** introduced by a model should be given by

\[
H^\Omega = \min \left\{ \frac{\nu \| \Delta u \|^2}{4|\tilde{R}|}, 1 \right\}
\]

where \( \tilde{R} = \int_\Omega R d\Omega \).
Stopping the vortex-stretching

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Notice that any model based on this ratio automatically **switches off** for:
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- Laminar flows \((R \to 0)\)
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Notice that any model based on this ratio automatically **switches off** for:

- Laminar flows (\( R \to 0 \))
- 2D flows (\( \lambda_2 = 0 \to R = 0 \))
- In the wall (near-wall behavior is given by \( R \propto y^1 \) and \( \| \Delta u \|^2 \propto y^0 \))
Stopping the vortex-stretching

The overall damping introduced by a model should be given by

\[ H^\Omega = \min \left\{ \frac{\nu \| \Delta u \|^2}{4|\tilde{R}|}, 1 \right\} \]

Stopping the vortex-stretching

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

\[
\nu_t \approx \frac{4|\tilde{R}|}{\| \Delta u \|^2}
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Stopping the vortex-stretching

The overall damping introduced by a model should be given by

\[ H^{\Omega} = \min \left\{ \nu \|\Delta u\|^2, \frac{4|\tilde{R}|}{\|\Delta u\|^2}, 1 \right\} \]

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

\[ \nu_t \approx \frac{4|\tilde{R}|}{\|\Delta u\|^2} \]

Taking \( \|\Delta u\|^2 \leq -\lambda_{\Delta}(\omega,\omega) = 4\lambda_{\Delta}\tilde{Q} \), it becomes the eddy-viscosity model\(^3\) based on the invariants \( R = -1/3tr(S^3) = -det(S) \) and \( Q = -1/2tr(S^2) \).

\( \lambda_{\Delta} < 0 \) is the largest (smallest in absolute value) non-zero eigenvalue of Laplacian operator \( \Delta \) on \( \Omega \). In a periodic box of size \( h \), \( \lambda_{\Delta} = -(\pi/h)^2 \).

Stopping the vortex-stretching

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

\[ f^{\text{reg}} \approx \min \left\{ \frac{\nu \| \Delta u \|}{4|\tilde{R}|}, 1 \right\} \]
**Stopping the vortex-stretching**

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**Or a combination of both?**
Towards a simple LES model

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

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

\[
\tau(\bar{u}) = -2\nu_t S(\bar{u})
\]
Towards a simple LES model

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

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

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

has been derived from the criterion that vortex-stretching mechanism must stop at the smallest grid scale

\[
\nu_t \approx \frac{4|\widetilde{R}|}{||\Delta \bar{u}||^2}
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Towards a simple LES model

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

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\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
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\]

And what about the implementation?

- No problems with \(4|\tilde{R}|\) and \(||\Delta \bar{u}||^2\).
Towards a simple LES model

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

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

And what about the implementation?

- No problems with \(4|\tilde{R}|\) and \(||\Delta \bar{u}||^2\).
- But, what about the **discretization** of \(\nabla \cdot \tau(\bar{u})\)?
A new simple approach to discretize the viscous term for eddy-viscosity models

\[
\begin{align*}
\partial_t u + C(u, u) &= \mathcal{D}u - \nabla p \\
\Omega_s \frac{d u_s}{d t} + C(u_s) u_s &= \mathcal{D}u_s + M^T p_c
\end{align*}
\]

\[\nabla \cdot u = 0, \quad \nabla \cdot u_s = 0_c\]
A new simple approach to discretize the viscous term for eddy-viscosity models

\[ \partial_t u + C(u, u) = D u - \nabla p + 2 \nabla \cdot (\nu_t S(u)), \quad \nabla \cdot u = 0 \]
\[ \Omega_s \frac{d u_s}{d t} + C(u_s) u_s = D u_s + M^T p_c \]

where \( 2 \nabla \cdot (\nu_t S(u)) = \nabla \cdot (\nu_t \nabla u) + \nabla \cdot (\nu_t \nabla u^T) \).
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\partial_t u + C(u, u) = D u - \nabla p + 2 \nabla \cdot (\nu_t S(u)), \quad \nabla \cdot u = 0
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\[
\Omega_s \frac{d u_s}{d t} + C(u_s) u_s = D u_s + M^T p_c + ??????, \quad M u_s = 0_c
\]

where \(2 \nabla \cdot (\nu_t S(u)) = \nabla \cdot (\nu_t \nabla u) + \nabla \cdot (\nu_t \nabla u^T).\)
A new simple approach to discretize the viscous term for eddy-viscosity models

\[
\partial_t u + C(u, u) = \mathcal{D} u - \nabla p + 2 \nabla \cdot (\nu_t S(u)), \quad \nabla \cdot u = 0
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\[
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\[ \nabla \cdot (\nu_t \nabla u^T) = \nabla (\nabla \cdot (\nu_t u)) - \nabla \cdot (u \otimes \nabla \nu_t) \]
A new simple approach to discretize the viscous term for eddy-viscosity models

\[
\partial_t u + C(u, u) = Du - \nabla p + 2\nabla \cdot (\nu_t S(u)), \quad \nabla \cdot u = 0
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\[
\nabla \cdot (\nu_t \nabla u^T) = \nabla(\nabla \cdot (\nu_t u)) - \nabla \cdot (u \otimes \nabla \nu_t)
\]

\[
= \nabla(\nabla \cdot (\nu_t u)) - C(u, \nabla \nu_t)
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A new simple approach to discretize the viscous term for eddy-viscosity models

\[
\begin{align*}
\partial_t u + C(u, u) &= D u - \nabla p + 2 \nabla \cdot (\nu_t S(u)), \quad \nabla \cdot u = 0 \\
\Omega_s \frac{d u_s}{d t} + C(u_s) u_s &= D u_s + M^T p_c + ????, \quad M u_s = 0_c
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where \(2 \nabla \cdot (\nu_t S(u)) = \nabla \cdot (\nu_t \nabla u) + \nabla \cdot (\nu_t \nabla u^T)\).

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

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

where \([\tilde{u}_s]_f = [\nu_{t,s}]_f [u_s]_f\). **Straightforward implementation!!!**
A new simple approach to discretize the viscous term for eddy-viscosity models

MMS for a fourth-order staggered formulation
Preliminary results

Turbulent channel flow

$Re_T = 590$  
DNS Moser et al.  
LES $64^3$

mean velocity  

rms fluctuations
Preliminary results

Turbulent square duct

\[ Re_\tau = 300 \]

\[ LES \; 64 \times 32 \times 32 \]

mean velocity

rms fluctuations

LES and regularization of turbulence
Conclusions

- The ratio between the invariant \( R \) and the (total) dissipation provides a proper differential operator for turbulence models.
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- Based on this, a new eddy-viscosity type LES models has been derived.
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- A simple new approach to discretize the viscous term for eddy-viscosity models has been proposed.
Conclusions and Future Research

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- Based on this, a new eddy-viscosity type LES models has been derived.
- 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 other configurations.
Conclusions and Future Research

- The ratio between the invariant $R$ and the (total) dissipation provides a proper differential operator for turbulence models.
- Based on this, a new eddy-viscosity type LES models has been derived.
- 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 other configurations.
- Try to properly combine regularization modeling and LES.
Thank you for your attention
Further reading

