Numerical simulation of turbulence at lower costs: regularization modeling

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DNS of turbulent incompressible flows on MareNostrum

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

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 on MareNostrum

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

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

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

Plane impingement jet at $Re = 20000$ (102M grid points)
Scaling? Yes\(^1\), we can... but never enough

\[256 \times 800 \times 1600 \ (327.7M)\]
\[256 \times 1400 \times 2800 \ (1003.5M)\]

Linear Speedup

70% efficiency

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

\[
D(\phi) = \nu \Delta \phi
\]
As the full energy spectrum cannot be computed, a dynamically less complex mathematical formulation is sought. We consider smooth approximations (regularizations) of the nonlinearity,

\[
\partial_t u_\epsilon + \tilde{\mathcal{C}}(u_\epsilon, u_\epsilon) = \mathcal{D}(u_\epsilon) - \nabla p_\epsilon
\]

such approximations may fall in the Large-Eddy Simulation (LES) concept,

\[
\partial_t \bar{u}_\epsilon + \mathcal{C}(\bar{u}_\epsilon, \bar{u}_\epsilon) = \mathcal{D}(\bar{u}_\epsilon) - \nabla \bar{p}_\epsilon + \mathcal{M}_1(\bar{u}_\epsilon, \bar{u}_\epsilon)
\]

if the filter is invertible:

\[
\mathcal{M}_1(\bar{u}_\epsilon, \bar{u}_\epsilon) = \mathcal{C}(\bar{u}_\epsilon, \bar{u}_\epsilon) - \tilde{\mathcal{C}}(u_\epsilon, u_\epsilon)
\]
Previous regularization modelings

Leray and Navier-Stokes-\(\alpha\) models

The regularization methods basically **alters the convective term** to **restrain the production of small scales** of motion.

- Leray model:

\[
\partial_t u_\epsilon + C(\bar{u}_\epsilon, u_\epsilon) = D(u_\epsilon) - \nabla p_\epsilon
\]

- Navier-Stokes-\(\alpha\) model:

\[
\partial_t u_\epsilon + C_r(u_\epsilon, \bar{u}_\epsilon) = D(u_\epsilon) - \nabla \pi_\epsilon
\]

where the \(\pi = p + u^2/2\) and the convective operator in rotational form is defined as \(C_r(u, v) = (\nabla \times u) \times v\)

However, in doing so some of the **inviscid invariants** (kinetic energy, enstrophy in 2D and helicity in 3D) are **not conserved**.
Symmetry-preserving regularization models (1/2)

In order to conserve the following inviscid invariants

- Kinetic energy : \((u, u)\)
- Enstrophy (in 2D) : \((\omega, \omega)\)
- Helicity (in 3D) : \((\omega, u)\)

where \((a, b) = \int_{\Omega} a \cdot b d\Omega\) and \(\omega = \nabla \times u\); the approximate convective operator must be skew-symmetric:

\[
(\tilde{C}(u, \phi_1), \phi_2) = - (\tilde{C}(u, \phi_2), \phi_1)
\]
Symmetry-preserving regularization models (2/2)

This criterion yields the following class of approximations\(^2\),

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

in which the convective term is smoothed according to:

\[
\begin{align*}
C_2(u, \phi) &= \overline{C(\bar{u}, \bar{\phi})} \\
C_4(u, \phi) &= C(\bar{u}, \bar{\phi}) + \overline{C(\bar{u}, \phi')} + \overline{C(u', \bar{\phi})} \\
C_6(u, \phi) &= C(\bar{u}, \bar{\phi}) + C(\bar{u}, \phi') + C(u', \bar{\phi}) + \overline{C(u', \phi')}
\end{align*}
\]

where \(u' = u - \bar{u}\) and \(C_n(u, \phi) = C(u, \phi) + O(\epsilon^n)\) for any symmetric filter.

Discretizing the $C_n$ regularization modeling

The regularizations $C_n$ are constructed in a way that the symmetry properties are exactly preserved.

Of course, the same should hold for the numerical approximations.

For this the basic ingredients are twofold:

- A symmetry-preserving spatial discretization of the original NS equations.
- A normalized self-adjoint linear filter.
Symmetry-preserving discretization of NS equations

The spatially discrete incompressible Navier-Stokes equations read

$$\Omega_s \frac{du_s}{dt} + C(u_s)u_s = Du_s - \Omega_s G p_c; \quad Mu_s = 0_c$$

Symmetries of underlying continuous operators must be preserved!

$$C = -C^T \quad \rightarrow \quad u_s^T Cu_s = 0 \quad \text{and} \quad \lambda_C \in \mathbb{I}$$

no false dissipation, only transport!

$$D = D^T \quad \text{def} - \quad u_s^T Du_s < 0 \quad \text{and} \quad D\hat{u}_k = \lambda_D \hat{u}_k, \quad \lambda_D \in \mathbb{R}^-$$

pure diffusion, no transport!

$$\Omega_s G = M^T \quad \rightarrow \quad -u_s^T \Omega_s G p_c = 0$$

no contribution to total kinetic energy!

to preserve the continuous inviscid invariants in a discrete sense.
Discrete filtering

Basic properties

\( \overline{u_s} = F u_s \)

Four properties are required:

i) Symmetry, \( \Omega_s F = (\Omega_s F)^T \)

ii) \( M u_s = 0_c \) \( \rightarrow \) \( M F u_s = 0_c \)

iii) Normalization, \( F 1 = 1 \)

iv) ... and of course, it must effectively damp the high-frequency components. **But, how much?**
Stopping the vortex-stretching\(^3\)

Taking the curl of momentum equation the vorticity transport equation follows

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

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

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

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

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

\(^3\)F.X. Trias et al. Computers\&Fluids, 39:1815-1831, 2010
Stopping the vortex-stretching

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

\[ (\omega, C(\omega, u)) = 4 \int_{\Omega} r \, d\Omega \quad (1) \]

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

\[ (\omega, \omega) = -4 \int_{\Omega} q \, d\Omega \]

Then, the diffusive term can be bounded by

\[ \nu (\nabla \omega, \nabla \omega) = -\nu (\omega, \Delta \omega) \leq -\nu \lambda_\Delta (\omega, \omega) = 4\nu \lambda_\Delta \int_{\Omega} q \, d\Omega \quad (2) \]

where \( \lambda_\Delta < 0 \) is the largest (smallest in absolute value) non-zero eigenvalue of Laplacian operator \( \Delta \) on \( \Omega \). If we now consider that the domain is a periodic box of volume \( h \), then \( \lambda_\Delta = -\left(\frac{\pi}{h}\right)^2 \).
Stopping the vortex stretching

In the present work we determine the filter width $\epsilon$ from

$$(\omega, C_4(\omega, u)) \approx f_4(\hat{g}_k(\epsilon))(\omega, C(\omega, u)) \leq \nu (\nabla \omega, \nabla \omega)$$

Then, recalling identity (1) and inequality (2), we propose to rewrite the previous inequality in terms of the invariants $q$ and $r$

$$f_4(\hat{g}_k) = \min \left\{ \nu \lambda_\Delta \frac{q}{r^+}, 1 \right\} \quad \text{with} \quad r^+ = \max(r, 0)$$

Notice that $q < 0$ (dissipation) whereas $r$ can be either positive or negative.

- Switches off ($f_4 = 1$) for: laminar ($r \to 0$), 2D flows ($r = 0$) and for fine enough meshes, $|\nu \lambda_\Delta q/r| \geq 1$.
- Consistent near-wall behavior $r \propto y^3$ and $q \propto y^0$.
- Consistent with the preferential vorticity alignment with the intermediate eigenvector, $\lambda_2$ (experimentally observed)
Test-case: Differentially Heated Cavity

Boundary conditions:

- **Isothermal vertical walls**
- **Adiabatic horizontal walls**
- **Periodic** boundary conditions in the spanwise direction

Dimensionless governing numbers:

- $Ra = \frac{\beta \Delta TL_z^3 g}{(\alpha \nu)}$
- $Pr = \frac{\nu}{\alpha}$
- Height aspect ratio $A_z = \frac{L_z}{L_y}$
- Depth aspect ratio $A_x = \frac{L_x}{L_y}$
DNS\textsuperscript{4,5} results for $Ra = 10^{11}$, $Pr = 0.71$

Some details about DNS:

- Mesh size: $128 \times 682 \times 1278$
- $\approx 3$ months - 256 CPUs
- $4^{th}$-order symmetry-preserving scheme
- $A_z = 4$

Complexity of the flow:

- Boundary layers
- Stratified cavity core
- Internal waves
- Recirculation areas

Results for differentially heated cavity at $Ra = 10^{11}$

- Regularization model $C_4$ is tested.
- Two coarse meshes are considered

<table>
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<tr>
<th></th>
<th>DNS</th>
<th>RM1</th>
<th>RM2</th>
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<tr>
<td>$Nz$</td>
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<td>85</td>
<td>56</td>
</tr>
</tbody>
</table>

- The **discrete linear filter**\(^6\) is based on polynomial functions of the discrete diffusive operator, $D$

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Results for differentially heated cavity at $Ra = 10^{11}$

Profiles

Averaged vertical velocity and temperature profiles at the horizontal mid-height plane.
How does the parameter-free $\tilde{C}_4$ regularization modeling behave for other grids and $Ra$-numbers?

Averaged vertical velocity and temperature profiles at the horizontal mid-height plane at $Ra = 10^{10}$.

Even for a **very coarse** $8 \times 13 \times 30$ grid **reasonable results** are obtained!

$\Rightarrow$ Results for different grids show the **robustness** of the method.
The overall Nusselt number and the centerline stratification for 50 randomly generated coarse grids with fixed stretching at $Ra = 10^{10}$. 

$8 \leq N_x \leq 16$, $17 \leq N_y \leq 34$, and $40 \leq N_z \leq 80$. 
Meshes have been generated with the criteria of keeping the same number of points in the BL than for $Ra = 10^{10}$. 
Conclusions and Future Research

The results shown illustrate the potential of the conservative parameter-free $\tilde{\mathcal{C}}_4$ smoothing as a new simulation shortcut.

The main advantages with respect exiting LES models can be summarized:

- **Robustness.** As the smoothed governing equations preserve the symmetry properties of the original NS equations the solution cannot blow up (in the energy-norm, in 2D also: enstrophy-norm). It seems that even for very coarse meshes reasonably results can be obtained.

- **Universality.** No *ad hoc* phenomenological arguments that cannot be formally derived for the NS equations are used.

- The proposed method constitutes a **parameter-free turbulence model**.
Thank you for your attention
Further reading about $C_4$ regularization

