Numerical simulation of turbulence at lower costs: regularization modeling

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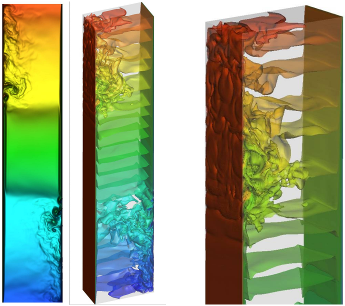
Contents

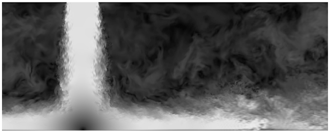
DNS of turbulent incompressible flows on MareNostrum

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

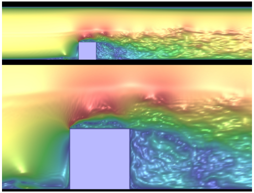


Air-filled differentially heated cavity at $Ra = 10^{11}$ (111M grid points)

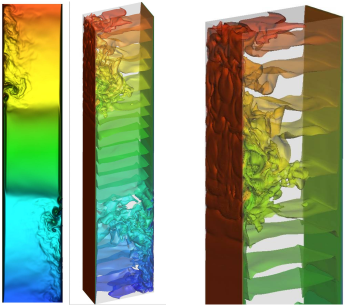


Plane impingement jet at $Re = 20000$ (102M grid points)

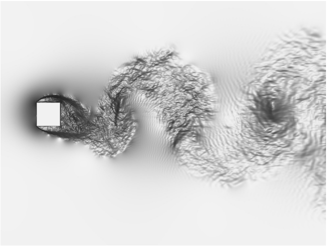
DNS of turbulent incompressible flows on MareNostrum



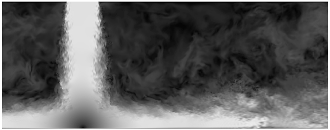
Wall-mounted cube at $Re = 7240$ (17M grid points)



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

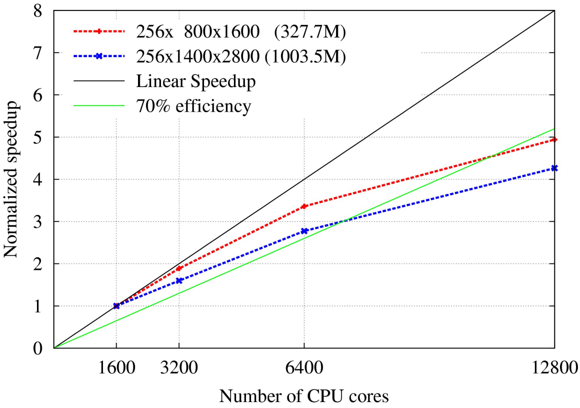


Square cylinder at $Re = 22000$ (75M grid points)



Plane impingement jet at $Re = 20000$ (102M grid points)

Scaling? Yes[1], we can... but never enough



[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:

$$\begin{aligned} \nabla \cdot u &= 0 \\ \partial_t u + \mathcal{C}(u,u) &= \mathcal{D}(u) - \nabla p \end{aligned}$$

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

$$\mathcal{C}(u,\phi) = (u \cdot \nabla)\phi$$

and the linear dissipative term is given by

$$\mathcal{D}(\phi) = \nu \Delta \phi$$

Regularization modeling

As the full energy spectrum cannot be computed, a **dynamically less complex mathematical formulation** is sought. We consider smooth approximations (regularizations) of the nonlinearity,

$$\partial_t u_\epsilon + \widetilde{\mathcal{C}}(u_\epsilon, u_\epsilon) = \mathcal{D}(u_\epsilon) - \nabla p_\epsilon$$

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:

$$\mathcal{M}_1(\bar{u}_\epsilon, \bar{u}_\epsilon) = \mathcal{C}(\bar{u}_\epsilon, \bar{u}_\epsilon) - \overline{\widetilde{\mathcal{C}}(u_\epsilon, u_\epsilon)}$$

Previous regularization modelings

Leray and Navier-Stokes-α models

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

- Leray model:

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

- Navier-Stokes-α model:

$$\partial_t u_\epsilon + \mathcal{C}_r(u_\epsilon, \bar{u}_\epsilon) = \mathcal{D}(u_\epsilon) - \nabla \pi_\epsilon$$

  where the $\pi = p + u^2/2$ and the convective operator in rotational form is defined as $\mathcal{C}_r(u, v) = (\nabla \times u) \times v$

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) : (ω, ω)
- Helicity (in 3D) : (ω, u)

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

$$\left(\widetilde{\mathcal{C}}(u, \phi_1), \phi_2\right) = -\left(\widetilde{\mathcal{C}}(u, \phi_2), \phi_1\right)$$

Symmetry-preserving regularization models (2/2)

This criterion yields the following class of approximations[2],

$$\partial_t u_\epsilon + \mathcal{C}_n(u_\epsilon, u_\epsilon) = \mathcal{D}(u_\epsilon) - \nabla p_\epsilon$$

in which the convective term in smoothed according to:

$$\begin{aligned}
\mathcal{C}_2(u,\phi) &= \overline{\mathcal{C}(\bar{u},\bar{\phi})} \\
\mathcal{C}_4(u,\phi) &= \mathcal{C}(\bar{u},\bar{\phi}) + \overline{\mathcal{C}(\bar{u},\phi')} + \overline{\mathcal{C}(u',\bar{\phi})} \\
\mathcal{C}_6(u,\phi) &= \mathcal{C}(\bar{u},\bar{\phi}) + \mathcal{C}(\bar{u},\phi') + \mathcal{C}(u',\bar{\phi}) + \overline{\mathcal{C}(u',\phi')}
\end{aligned}$$

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

[2] Roel Verstappen, **Computers & Fluids**, 37 (7): 887-897, 2008

Discretizing the $\mathcal{C}_n$ regularization modeling

The regularizations $\mathcal{C}_n$ 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

$$\Omega_s \frac{d\boldsymbol{u}_s}{dt} + \mathsf{C}(\boldsymbol{u}_s)\boldsymbol{u}_s = \mathsf{D}\boldsymbol{u}_s - \Omega_s \mathsf{G}\boldsymbol{p}_c \; ; \qquad \mathsf{M}\boldsymbol{u}_s = \mathbf{0}_c$$

Symmetries of underlying continuous operators must be preserved!

$$\mathsf{C} = -\mathsf{C}^T \qquad \longrightarrow \qquad \boldsymbol{u}_s^T \mathsf{C} \boldsymbol{u}_s = 0 \quad \text{and} \quad \lambda_{\mathsf{C}} \in \mathbb{I}$$

no false dissipation, only transport!

$$\mathsf{D} = \mathsf{D}^T \quad def- \quad \longrightarrow \quad \boldsymbol{u}_s^T \mathsf{D} \boldsymbol{u}_s < 0 \;\; \text{and} \;\; \mathsf{D}\hat{\boldsymbol{u}}_k = \lambda_{\mathsf{D}} \hat{\boldsymbol{u}}_k \;,\; \lambda_{\mathsf{D}} \in \mathbb{R}^-$$

pure diffusion, no transport!

$$-\Omega_s \mathsf{G} = \mathsf{M}^T \qquad \longrightarrow \qquad -\boldsymbol{u}_s^T \Omega_s \mathsf{G} \boldsymbol{p}_c = 0$$

no contribution to total kinetic energy!

to **preserve** the continuous **inviscid invariants** in a **discrete** sense.

Discrete filtering

Basic properties

$$\overline{\boldsymbol{u}_s} = F\boldsymbol{u}_s$$

Four properties are required:

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

ii) $M\boldsymbol{u}_s = \boldsymbol{0}_c \longrightarrow MF\boldsymbol{u}_s = \boldsymbol{0}_c$

iii) Normalization, $F1 = 1$

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, Ω, 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 $r = -1/3tr(S^3)$

$$(\omega, \mathcal{C}(\omega, u)) = 4 \int_\Omega r d\Omega \qquad (1)$$

whereas the $L^2(\Omega)$-norm of ω in terms of the invariant $q = -1/2tr(S^2)$

$$(\omega, \omega) = -4 \int_\Omega q d\Omega$$

Then, the diffusive term can be bounded by

$$\nu (\nabla\omega, \nabla\omega) = -\nu (\omega, \Delta\omega) \leq -\nu\lambda_\Delta (\omega, \omega) = 4\nu\lambda_\Delta \int_\Omega q d\Omega \qquad (2)$$

where $\lambda_\Delta < 0$ is the largest (smallest in absolute value) non-zero eigenvalue of Laplacian operator Δ on Ω. If we now consider that the domain is a periodic box of volume h, then $\lambda_\Delta = -(\pi/h)^2$.

Stopping the vortex stretching

$\Longrightarrow$ In the present work we **determine the filter width** ϵ from

$$(\omega, \mathcal{C}_4(\omega, u)) \quad \approx \quad f_4(\hat{g}_k(\epsilon))(\omega, \mathcal{C}(\omega, u)) \quad \leq \quad \nu (\nabla\omega, \nabla\omega)$$

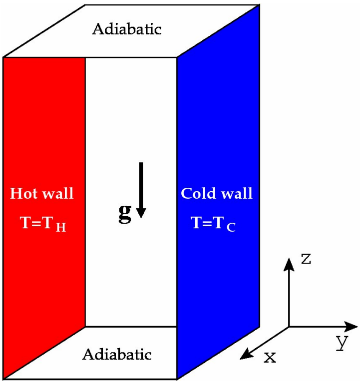
Then, recalling identity (1) and inequality (2), we propose to rewrite the previous inequality in terms of the invariants q and r

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

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, λ_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:

- $Ra = \beta \Delta T L_z^3 g/(\alpha\nu)$
- $Pr = \nu/\alpha$
- Height aspect ratio $A_z = L_z/L_y$
- Depth aspect ratio $A_x = L_x/L_y$

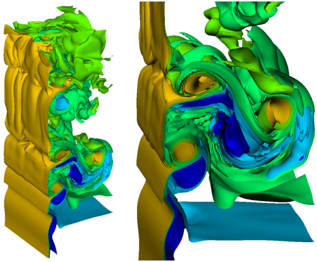
DNS[4,5] results for $Ra = 10^{11}$, $Pr = 0.71$

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



[4] F. X. Trias *et al.* Int. Journal of Heat and Mass Transfer, 53:665-673, 2010

[5] F. X. Trias *et al.* Int. Journal of Heat and Mass Transfer, 53:674-683, 2010

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

- Regularization model $\mathcal{C}_4$ is tested.
- Two coarse meshes are considered

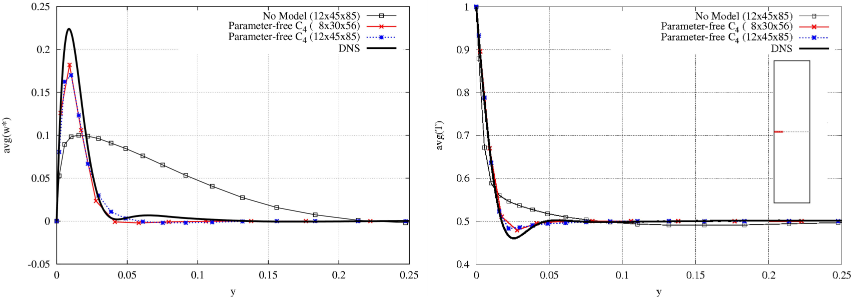
	DNS	RM1	RM2
Nx	128	12	8
Ny	682	45	30
Nz	1278	85	56

- The **discrete linear filter**[6] is based on polynomial functions of the discrete diffusive operator, D

[6] F.X. Trias and R.W.C.P. Verstappen, **Computers & Fluids**, 40:139-148, 2011

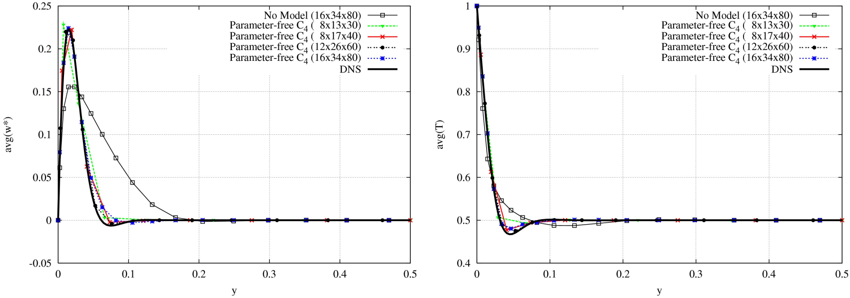
Results for differentially heated cavity at $Ra = 10^{11}$

Profiles



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

How does the parameter-free $\widetilde{\mathcal{C}}_4$ regularization modeling behave for other grids and *Ra*-numbers?

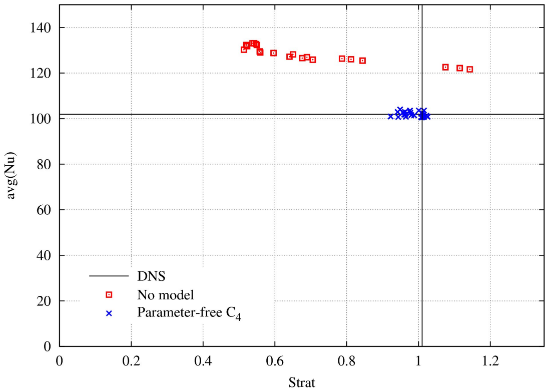


Averaged vertical velocity and temperature profiles at the horizontal mid-height plane at $Ra = 10^{10}$.

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

$\Longrightarrow$ Results for different grids show the **robustness** of the method.

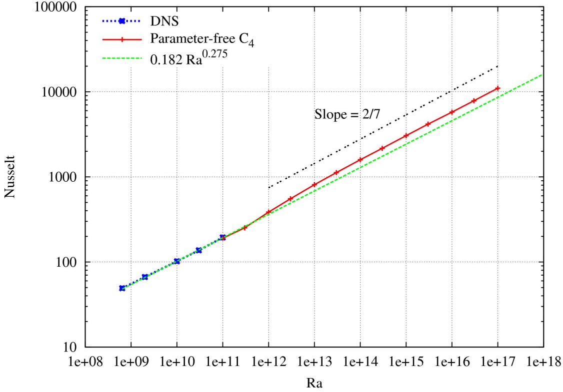
Challenging $\mathcal{C}_4$: mesh independence analysis



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 $40 \leq N_z \leq 80$.

Performance at very high Rayleigh numbers



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 $\widetilde{\mathcal{C}}_4$ smoothing as a new simulation shortcut.

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

- **Robustnest**. 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 you attention

Further reading about $\mathcal{C}_4$ regularization

- Roel Verstappen, *"On restraining the production of small scales of motion in a turbulent channel flow"*, Computers & Fluids, 37 (7): 887-897, 2008
- F. X. Trias *et al.*, *"Parameter-free symmetry-preserving regularization modeling of a turbulent differentially heated cavity"*, Computers & Fluids, 39:1815-1831, 2010.
- F. X. Trias and R.W.C.P. Verstappen, *"On the construction of discrete filters for symmetry-preserving regularization models"*, Computers & Fluids, 40:139-148, 2011.