New discretizations and regularization models for LES

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

26^{th} International Conference on Parallel Computational Fluid Dynamics

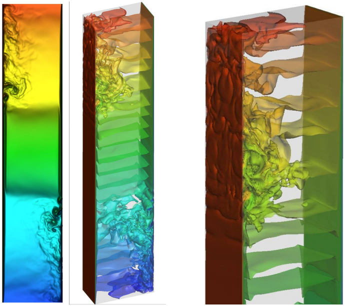
Trondheim (Norway), May 20-22 2014

Contents

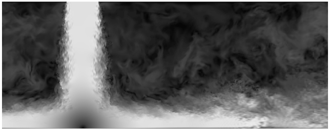
DNS of turbulent incompressible flows

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

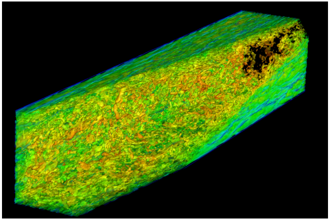


Air-filled differentially heated cavity at $Ra = 10^{11}$ (111M grid points)

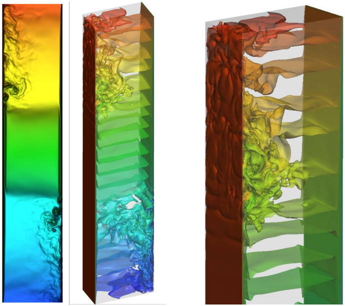


Plane impingement jet at $Re = 20000$ (102M grid points)

DNS of turbulent incompressible flows



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



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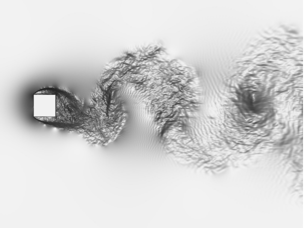
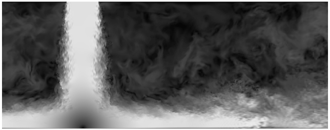
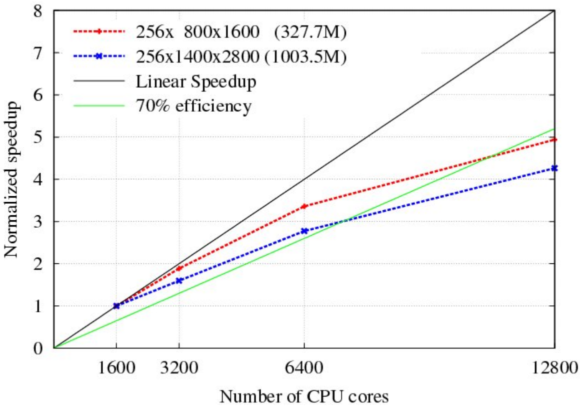


Square cylinder at $Re = 22000$ (300M grid points)



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

Scaling is possible[1]... 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**, 49:101-109, 2011

Governing equations

Incompressible Navier-Stokes equations:

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

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

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

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

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

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

Symmetry-preserving regularization modeling

We consider smooth approximations (regularizations) of the nonlinearity,

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

that conserve the following inviscid invariants

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

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The **approximate convective operator** must **preserve** the basic **symmetry** properties:

$$(\mathcal{C}(u, v), \quad w) = -(\mathcal{C}(u, \quad w), v)$$
$$(\mathcal{C}(u, v), \Delta v) = \quad (\mathcal{C}(u, \Delta v), v) \qquad \text{in 2D}$$

Symmetry-preserving regularization models

Regularizations of the non-linear convectiver term can be constructed

$$\tilde{\mathcal{C}}(u,v) = \sum_{i,j,k=0}^{1} a_{ijk}\tilde{\mathcal{C}}_{ijk}(u,v)$$

where $\tilde{\mathcal{C}}_{ijk}(u,v) = \varphi_k\left(\mathcal{C}(\varphi_i(u),\varphi_j(v))\right)$ and $\varphi_i(u) = \begin{cases} u\ , & \text{if } i=0 \\ \overline{u}\ , & \text{if } i=1 \end{cases}$

$\overline{(\cdot)}$ is a **self-adjoint** filter that **commutes** with differential operators.

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Among all possible combinations we find the regularization proposed by Leray, $\mathcal{C}(\overline{u}, u)$: $a_{100} = 1$ (with the rest of $a_{ijk} = 0$)

$\Longrightarrow$ Eight coefficients a_{ijk} need to be determined.

Symmetry-preserving regularization models

$$\tilde{\mathcal{C}}(u,v) = \sum_{i,j,k=0}^{1} a_{ijk}\tilde{\mathcal{C}}_{ijk}(u,v)$$

$$\sum_{i,j,k=0}^{1} a_{ijk} = 1 \quad \longrightarrow \quad \tilde{\mathcal{C}}(u,v) = \mathcal{C}(u,v) + \mathcal{O}(\epsilon^n) \quad \text{with } n \geq 2$$

$$\left(\tilde{\mathcal{C}}(u,v),\ w\right) = -\left(\tilde{\mathcal{C}}(u,\ w), v\right) \quad \longrightarrow \quad a_{ijk} = a_{ikj}$$

$$\left(\tilde{\mathcal{C}}(u,v), \Delta v\right) = \left(\tilde{\mathcal{C}}(u,\Delta v), v\right) \quad \text{in 2D} \quad \longrightarrow \quad a_{ijk} = a_{kji}$$

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

Symmetry-preserving regularization models

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This leads to a family of $\mathcal{O}(\epsilon^2)$-accurate regularizations. Among them[2],

$$\boxed{\mathcal{C}_2(u,v) = \tilde{\mathcal{C}}_{111}(u,v) = \overline{\mathcal{C}(\overline{u},\overline{v})}}$$

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

Symmetry-preserving regularization models

To cancel second-order terms, three additional conditions need to imposed:

$$\sum_{j,k=0}^{1} a_{1jk} = 0 \qquad \sum_{i,k=0}^{1} a_{i1k} = 0 \qquad \sum_{i,j=0}^{1} a_{ij1} = 0$$

$$\boxed{\mathcal{C}_4^{\gamma}(u,v) = \frac{1}{2}\left((\mathcal{C}_4 + \mathcal{C}_6) + \gamma(\mathcal{C}_4 - \mathcal{C}_6)\right)(u,v)}$$

where $\mathcal{C}_4$ and $\mathcal{C}_6$ read

$$\mathcal{C}_4(u,v) = \mathcal{C}(\bar{u},\bar{v}) + \overline{\mathcal{C}(\bar{u},v')} + \overline{\mathcal{C}(u',\bar{v})}$$
$$\mathcal{C}_6(u,v) = \mathcal{C}(\bar{u},\bar{v}) + \mathcal{C}(\bar{u},v') + \mathcal{C}(u',\bar{v}) + \overline{\mathcal{C}(u',v')}$$

Symmetry-preserving regularization models

Taking $\gamma = 1$ we obtain the $\mathcal{C}_4$ approximation[2],

$$\partial_t u_\epsilon + \mathcal{C}_4(u_\epsilon, u_\epsilon) = \mathcal{D}(u_\epsilon) - \nabla p_\epsilon$$

in which the convective term in smoothed according to:

$$\boxed{\mathcal{C}_4(u, v) = \mathcal{C}(\bar{u}, \bar{v}) + \overline{\mathcal{C}(\bar{u}, v')} + \overline{\mathcal{C}(u', \bar{v})}}$$

where $u' = u - \bar{u}$ and $\mathcal{C}_4(u, v) = \mathcal{C}(u, v) + \mathcal{O}(\epsilon^4)$ for **any symmetric filter**.

High-frequencies need to be effectively damped.

But how much?

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

Symmetry-preserving regularization models

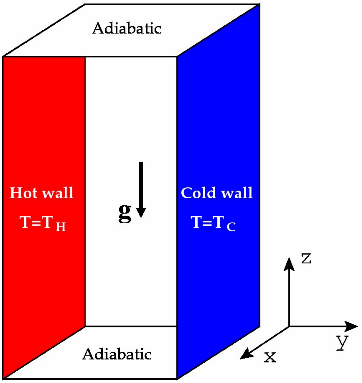
Answer: Again the balance between vortex-stretching contribution and physical dissipation provides a proper value for the damping

$$f_4(\hat{g}_k(\epsilon)) \approx \min\left\{\frac{\nu\|\Delta u\|^2}{4|\widetilde{R}|}, 1\right\}$$

where

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

Test-case: Differentially Heated Cavity



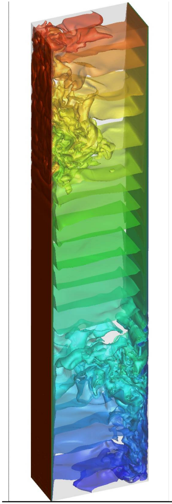
Boundary conditions:

- **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[3,4] results for $Ra = 10^{11}$, $Pr = 0.71$

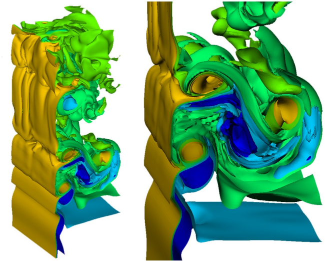


Some details about **DNS**:

- 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



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

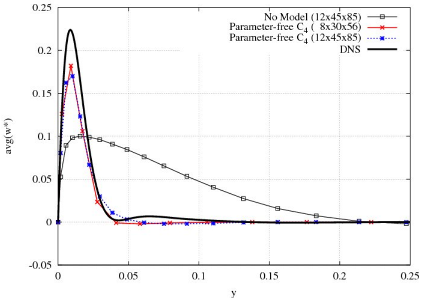
	DNS	RM1	RM2
Nx	128	12	8
Ny	682	45	30
Nz	1278	85	56

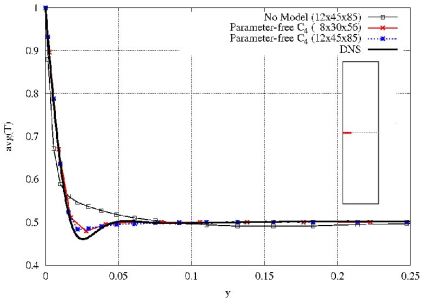
- The **discrete linear filter**[5] is based on polynomial functions of the discrete diffusive operator, D

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

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

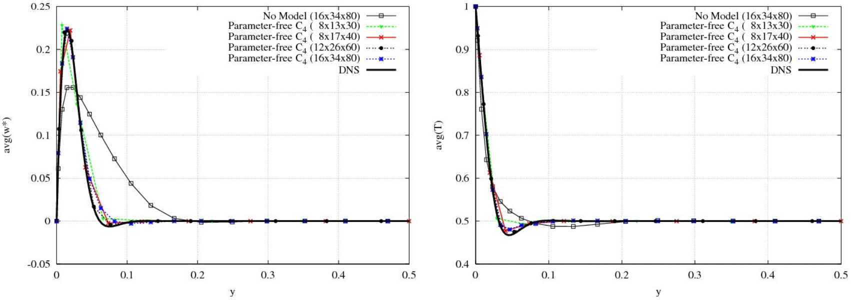
Profiles





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?

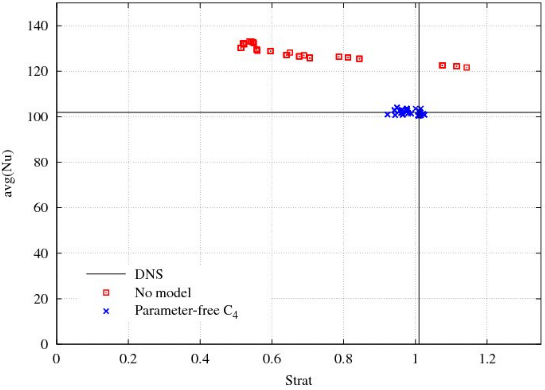


Averaged vertical velocity and temperature profiles at the horizontal mid-height plane at $Ra = 10^{10}$.

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 $40 \leq N_z \leq 80$.

Towards a simple LES model

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

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

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

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

$$\boxed{\nu_t \approx \frac{4|\widetilde{R}|}{\|\Delta \overline{u}\|^2}}$$

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And what about the implementation?

- No problems with $4|\widetilde{R}|$ and $\|\Delta \overline{u}\|^2$.

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And what about the implementation?

- No problems with $4|\widetilde{R}|$ and $\|\Delta \overline{u}\|^2$.
- But, what about the **discretization** of $\nabla \cdot \tau(\overline{u})$?

Discretization of $2\nabla \cdot (\nu_t S(u))$: a new simple approach[6]

$$\partial_t u + \mathcal{C}(u, u) = \mathcal{D} u - \nabla p \quad , \quad \nabla \cdot u = 0$$

$$\Omega_s \frac{du_s}{dt} + \mathsf{C}(u_s) u_s = \mathsf{D} u_s + \mathsf{M}^T p_c \quad , \quad \mathsf{M} u_s = 0_c$$

[6] F.X.Trias *et al. A simple approach to discretize the viscous term with spatially varying (eddy-)viscosity* **Journal of Computational Physics**, 253:405-417, 2013

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$$\boxed{\underbrace{-\mathsf{M}^T \Omega_c^{-1} \mathsf{M} \tilde{u}_s}_{\approx \nabla(\nabla \cdot (\nu_t u))} - \underbrace{\mathsf{C}(u_s)(-\Omega_s^{-1} \mathsf{M}^T \nu_{t,c})}_{\approx \mathcal{C}(u, \nabla \nu_t)}}$$

where $[\tilde{u}_s]_f = [\nu_{t,s}]_f [u_s]_f$. **Straightforward implementation!!!**

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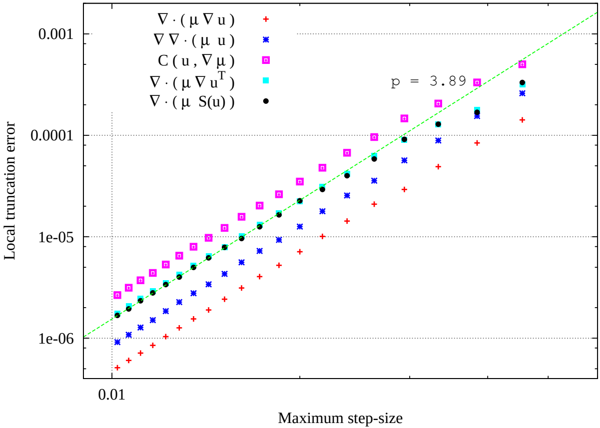
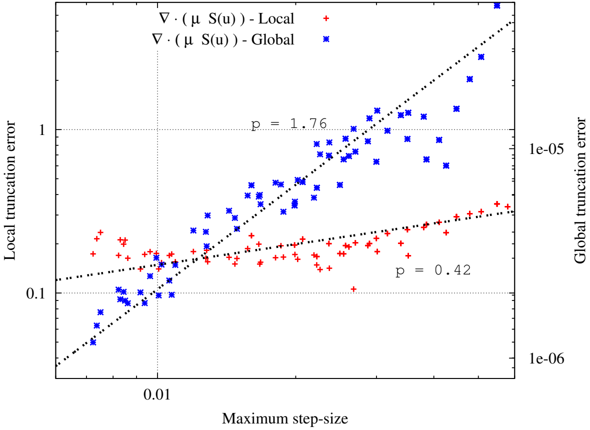
Discretization of $2\nabla \cdot (\nu_t S(u))$: a new simple approach

4^{th}-order FVM on a staggered Cartesian grid



Discretization of $2\nabla \cdot (\nu_t S(u))$: 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...

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$$\underbrace{-\mathsf{M}^T \Omega_c^{-1} \mathsf{M} \tilde{u}_s}_{\approx \nabla(\nabla \cdot (\nu_t u))} - \underbrace{\mathsf{C}(u_s)(-\Omega_s^{-1} \mathsf{M}^T \nu_{t,c})}_{\approx \mathcal{C}(u, \nabla \nu_t)}$$

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

Discretization of $2\nabla \cdot (\nu_t S(u))$: a new simple approach

Let's make it even easier...

$$\nabla \cdot (\nu_t \nabla u^T) = \nabla(\nabla \cdot (\nu_t u)) - \mathcal{C}(u, \nabla \nu_t)$$

$$\boxed{\underbrace{-\mathsf{M}^T \Omega_c^{-1} \mathsf{M} \tilde{u}_s}_{\approx \nabla(\nabla \cdot (\nu_t u))} - \underbrace{\mathsf{C}\,(u_s)(-\Omega_s^{-1} \mathsf{M}^T \nu_{t,c})}_{\approx \mathcal{C}(u, \nabla \nu_t)}}$$

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

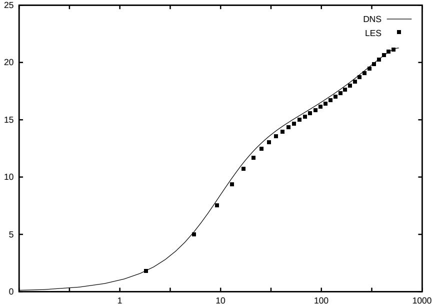
Therefore, the only term that needs to be discretized is

$$\boxed{-\underbrace{\mathsf{C}\,(u_s)(-\Omega_s^{-1} \mathsf{M}^T \nu_{t,c})}_{\approx \mathcal{C}(u, \nabla \nu_t)}}$$

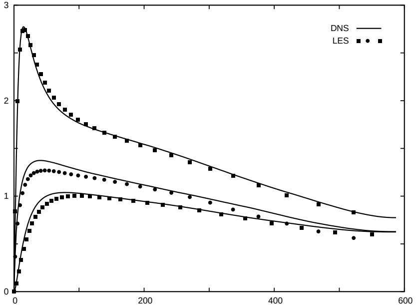
Preliminary results

Turbulent channel flow

$Re_\tau = 590$ DNS Moser et al. LES 64^3



mean velocity

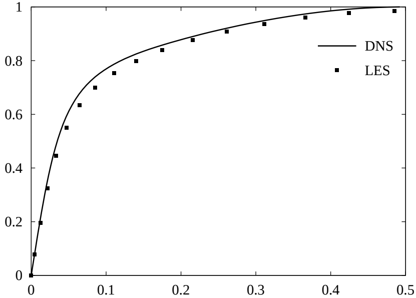


rms fluctuations

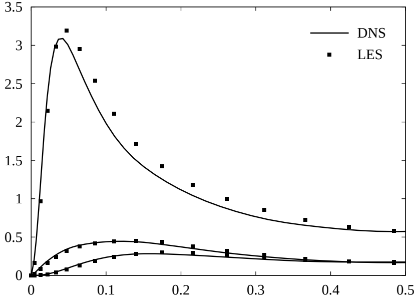
Preliminary results

Turbulent square duct

$Re_\tau = 300$ LES $64 \times 32 \times 32$



mean velocity



rms fluctuations

Conclusions

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Conclusions and Future Research

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

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- 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

- Roel Verstappen, *"When does eddy viscosity damp subfilter scales sufficiently?"*, Journal of Scientific Computing, 49 (1): 94-110, 2011
- F.X.Trias, R.W.C.P.Verstappen, A.Gorobets, M.Soria, A.Oliva, *"Parameter-free symmetry-preserving regularization modeling of a turbulent differentially heated cavity"*, Computers & Fluids, 39:1815-1831, 2010.
- F.X.Trias, A.Gorobets, A.Oliva, *A simple approach to discretize the viscous term with spatially varying (eddy-)viscosity*, Journal of Computational Physics, 253:405-417, 2013.