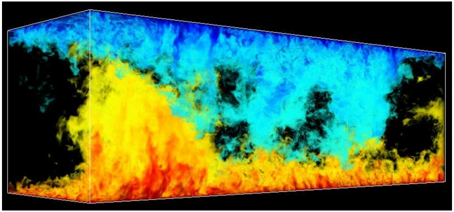
Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

Tackling turbulence with (super)computers at CTTC

F.Xavier Trias, Joaquim Rigola, Assensi Oliva

Heat and Mass Transfer Technological Center, Technical University of Catalonia



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Advanced models for large-eddy simulation of turbulent flows

F.Xavier Trias, Joaquim Rigola, Assensi Oliva

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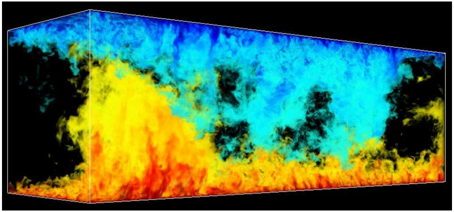
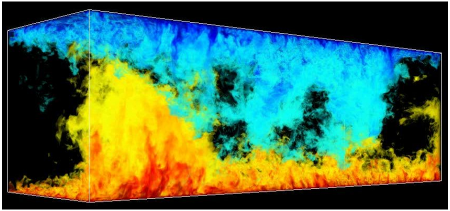


Contents

Motivation

Research question:

- Can we find a (nonlinear) SGS heat flux model with **good physical** and **numerical properties**, such that we can obtain satisfactory predictions for a turbulent Rayleigh-Bénard convection?



DNS of an air-filled Rayleigh-Bénard convection at $Ra = 10^{10}$

[1] F.Dabbagh, F.X.Trias, A.Gorobets, A.Oliva. *On the evolution of flow topology in turbulent Rayleigh-Bénard convection*, **Physics of Fluids**, 28:115105, 2016.

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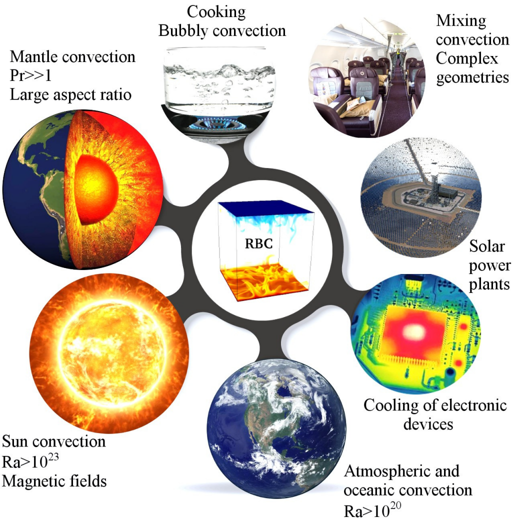
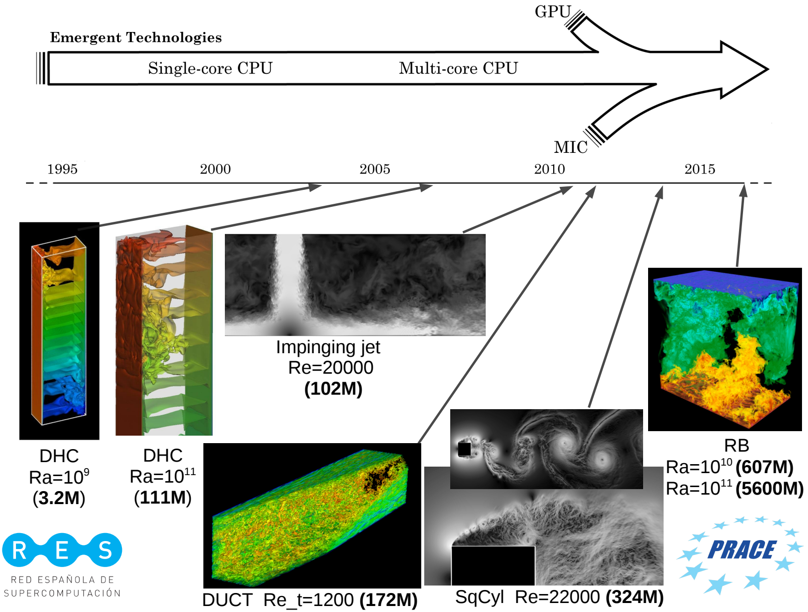

Cooking
Bubbly convection
Mixing
convection
Complex
geometries
Mantle convection
Pr>>1
Large aspect ratio
RBC
Solar
power
plants
Cooling of electronic
devices
Sun convection
Ra>10^23
Magnetic fields
Atmospheric and
oceanic convection
Ra>10^20

Motivation

And of course... saving the planet!


GPU
Emergent Technologies
Single-core CPU
Multi-core CPU
MIC
1995
2000
2005
2010
2015
Impinging jet
Re=20000
(102M)
RB
Ra=10^{10} **(607M)**
Ra=10^{11} **(5600M)**
DHC
Ra=10^{9}
(3.2M)
DHC
Ra=10^{11}
(111M)
RES
RED ESPAÑOLA DE SUPERCOMPUTACIÓN
DUCT Re_t=1200 **(172M)**
SqCyl Re=22000 **(324M)**
PRACE

Eddy-viscosity models for LES

$$\partial_t \overline{u} + (\overline{u} \cdot \nabla)\overline{u} = \nabla^2 \overline{u} - \nabla \overline{p} - \nabla \cdot \tau(\overline{u}) \quad ; \qquad \nabla \cdot \overline{u} = 0$$

$$\text{eddy-viscosity} \quad \longrightarrow \quad \tau\ (\overline{u}) = -2\nu_t S(\overline{u})$$

[2] F.X.Trias, D.Folch, A.Gorobets, A.Oliva. *Building proper invariants for eddy-viscosity subgrid-scale models*, **Physics of Fluids**, 27: 065103, 2015.

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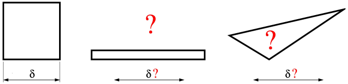

δ?

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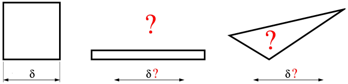

δ

[3] F.X.Trias, A.Gorobets, M.Silvis, R.Verstappen, A.Oliva. *A new subgrid characteristic length for turbulence simulations on anisotropic grids*, **Phys.Fluids**, 26:115109, 2017.

Building proper invariants for LES models

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Therefore, they can be characterized by 5 **basic invariants**

$$\boxed{\{Q_S, R_S, Q_G, R_G, V^2\}}$$

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Notation: given a second-order tensor A

First invariant: $P_A = tr(A)$
Second invariant: $Q_A = 1/2\{tr^2(A) - tr(A^2)\}$
Third invariant: $R_A = det(A)$

Building proper invariants for LES models

$$\partial_t \overline{u} + (\overline{u} \cdot \nabla)\overline{u} = \nabla^2 \overline{u} - \nabla \overline{p} - \nabla \cdot \tau(\overline{u}) \quad ; \qquad \nabla \cdot \overline{u} = 0$$

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Notation:

$$V^2 = 4(tr(S^2\Omega^2) - 2Q_S Q_\Omega),$$

where $S = 1/2(G + G^T)$ and $\Omega = 1/2(G - G^T)$.

A unified framework for eddy-viscosity models

$$\{Q_S, R_S, Q_G, R_G, V^2\}$$

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Sigma model $$\nu_t^{\sigma} = (C_\sigma\delta)^2\frac{\sigma_3(\sigma_1-\sigma_2)(\sigma_2-\sigma_3)}{\sigma_1^2},$$

where $\sigma_i = \sqrt{\lambda_i}$ and λ_i is an eigenvalue of GG^T.

Near-wall behavior

$$\{Q_S, R_S, Q_G, R_G, V^2\}$$

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$$\{Q_S, R_S, Q_G, R_G, V^2\}$$

	Invariants					
	Q_G	R_G	Q_S	R_S	V^2	Q_Ω
Wall-behavior	$\mathcal{O}(y^2)$	$\mathcal{O}(y^3)$	$\mathcal{O}(y^0)$	$\mathcal{O}(y^1)$	$\mathcal{O}(y^0)$	$\mathcal{O}(y^0)$
Units	$[T^{-2}]$	$[T^{-3}]$	$[T^{-2}]$	$[T^{-3}]$	$[T^{-4}]$	$[T^{-2}]$

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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[4]

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

$$\nu_t = (C_M \delta)^2 P^p_{GG^T} Q^q_{GG^T} R^r_{GG^T},$$

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$$-6r - 4q - 2p = -1; \qquad 6r + 2q = s,$$

where s is the slope for the asymptotic near-wall behavior, *i.e.* $\mathcal{O}(y^s)$.

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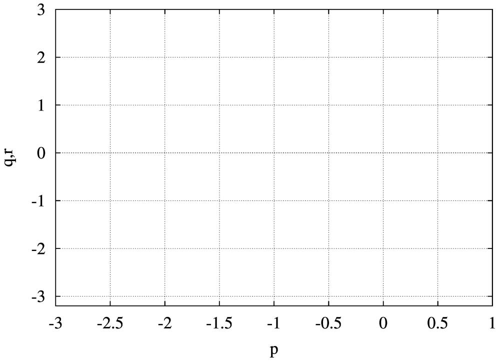
Solutions: $q(p, s) = (1 - s)/2 - p$ and $r(p, s) = (2s - 1)/6 + p/3$



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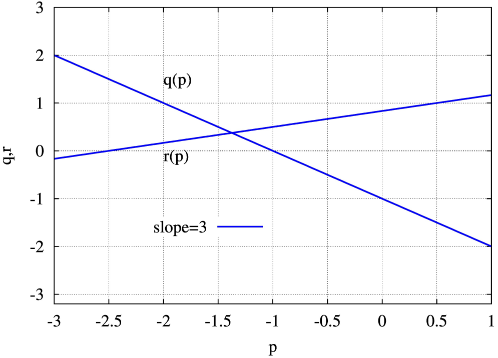

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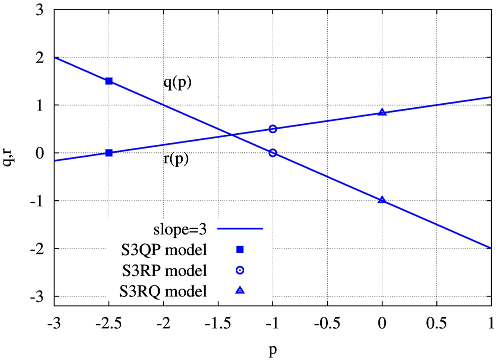

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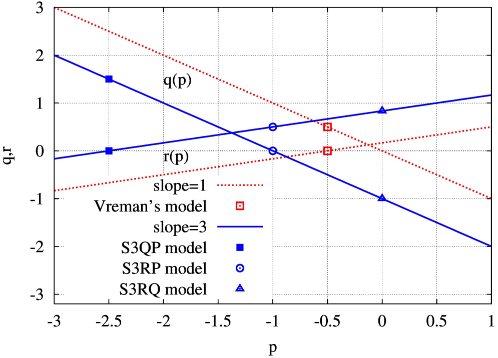

Building proper models for LES

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

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

$$\nu_t^{S3QP} = (C_{s3qp}\delta)^2 P_{GG^T}^{-5/2} Q_{GG^T}^{3/2},$$

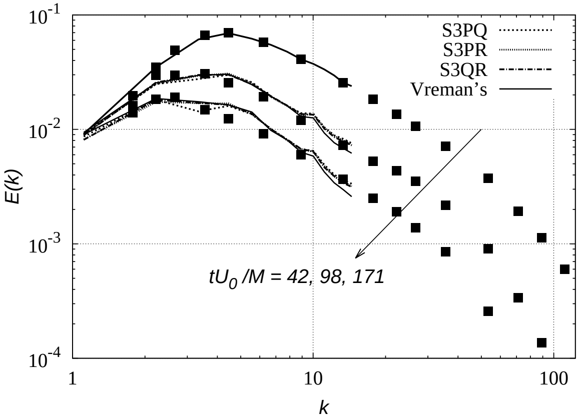
$$\nu_t^{S3RP} = (C_{s3rp}\delta)^2 P_{GG^T}^{-1} R_{GG^T}^{1/2},$$

$$\nu_t^{S3RQ} = (C_{s3rq}\delta)^2 Q_{GG^T}^{-1} R_{GG^T}^{5/6}.$$

Buiding proper models for LES

Decaying isotropic turbulence with $C_{s3pq} = 0.572$, $C_{s3pr} = 0.709$, $C_{s3qr} = 0.762$

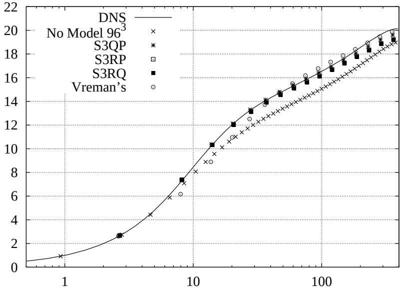
Comparison with classical Comte-Bellot & Corrsin (CBC) experiment.

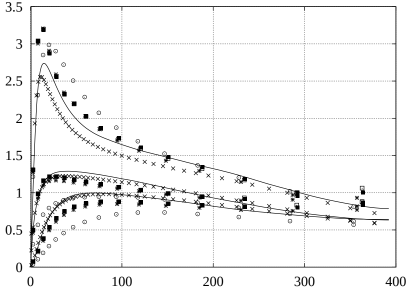


Turbulent channel flow

Results

$Re_\tau = 395$ DNS Moser et al. LES 32^3



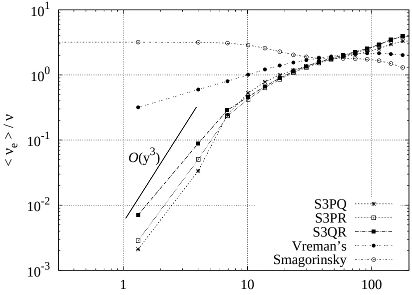


mean velocity

rms fluctuations

Turbulent channel flow

Near-wall behavior



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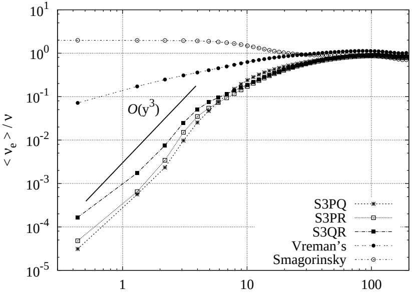

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PHYSICS OF FLUIDS **27**, 065103 (2015)

Building proper invariants for eddy-viscosity subgrid-scale models

F. X. Trias,[1,a)] D. Folch,[1,b)] A. Gorobets,[1,2,c)] and A. Oliva[1,d)]
[1]*Heat and Mass Transfer Technological Center, Technical University of Catalonia, ETSEIAT, c/Colom 11, 08222 Terrassa, Spain*
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Direct simulations of the incompressible Navier-Stokes equations are limited to relatively low-Reynolds numbers. Hence, dynamically less complex mathematical formulations are necessary for coarse-grain simulations. Eddy-viscosity models for large-eddy simulation is probably the most popular example thereof: they rely on differential operators that should properly detect different flow configurations (laminar and 2D flows, near-wall behavior, transitional regime, etc.). Most of them are based on the combination of invariants of a symmetric tensor that depends on the gradient of the resolved velocity field, $\mathsf{G} = \nabla \overline{\boldsymbol{u}}$. In this work, models are presented within a framework consisting of a 5D phase space of invariants. In this way, new models can be constructed by imposing appropriate restrictions in this space. For instance, considering the three invariants P_{GG^T}, Q_{GG^T}, and R_{GG^T} of the tensor GG^T, and imposing the proper cubic near-wall behavior, i.e., $\nu_e = \mathcal{O}(y^3)$, we deduce that the eddy-viscosity is given by $\nu_e = (C_{s3pqr}\Delta)^2 P^p_{\mathsf{GG}^T} Q^{-(p+1)}_{\mathsf{GG}^T} R^{(p+5/2)/3}_{\mathsf{GG}^T}$. Moreover, only R_{GG^T}-dependent models, i.e., $p > -5/2$, switch off for 2D flows. Finally, the model constant may be related with the Vreman's model constant via $C_{s3pqr} = \sqrt{3} C_{Vr} \approx 0.458$; this guarantees both numerical stability and that the models have less or equal dissipation than Vreman's model, i.e., $0 \le \nu_e \le \nu_e^{Vr}$. The performance of the proposed models is successfully tested for decaying isotropic turbulence and a turbulent channel flow. The former test-case has revealed that the model constant, C_{s3pqr}, should be higher than 0.458 to obtain the right amount of subgrid-scale dissipation, i.e., $C_{s3pq} = 0.572$ ($p = -5/2$), $C_{s3pr} = 0.709$ ($p = -1$), and $C_{s3qr} = 0.762$ ($p = 0$). © *2015 AIP Publishing LLC.* [http://dx.doi.org/10.1063/1.4921817]

Subgrid characteristic length for LES: state of the art

$$\partial_t \overline{u} + (\overline{u} \cdot \nabla)\overline{u} = \nabla^2 \overline{u} - \nabla \overline{p} - \nabla \cdot \tau(\overline{u}) \;\; ; \qquad \nabla \cdot \overline{u} = 0$$

$$\text{eddy-viscosity} \;\longrightarrow\; \tau\;(\overline{u}) = -2\nu_t S(\overline{u})$$

$$\boxed{\nu_t = (C_m \delta)^2 D_m(\overline{u})}$$

$D_m(\overline{u}) \longrightarrow$ Smagorinsky (1963), WALE (1999), Vreman (2004), QR-model (2011), σ-model (2011), S3PQR (2015)...

$C_m \longrightarrow$ Germano's dynamic model (1991), Lagrangian dynamic (1995), Global dynamic approach (2006)

[5] F.X.Trias, A.Gorobets, M.Silvis, R.Verstappen, A.Oliva. *A new subgrid characteristic length for turbulence simulations on anisotropic grids*, **Phys.Fluids**, 26:115109, 2017.

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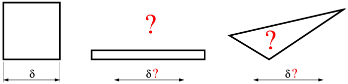

δ?

[5] F.X.Trias, A.Gorobets, M.Silvis, R.Verstappen, A.Oliva. *A new subgrid characteristic length for turbulence simulations on anisotropic grids*, **Phys.Fluids**, 26:115109, 2017.

Subgrid characteristic length for LES: state of the art

- In the context of **LES**, most popular (by far) is:

$$\boxed{\delta_{\mathrm{vol}} = (\Delta x \Delta y \Delta z)^{1/3}} \Longleftarrow \textbf{Deardorff (1970)}$$

$$\delta_{\mathrm{Sco}} = f(a_1, a_2)\delta_{\mathrm{vol}}, \qquad \delta_{L^2} = \sqrt{(\Delta x^2 + \Delta y^2 + \Delta z^2)/3}$$

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- In the context of **DES**:

$$\boxed{\delta_{\mathsf{max}} = \max(\Delta x, \Delta y, \Delta z)} \Longleftarrow \textbf{Sparlart et al. (1997)}$$

Recent flow-dependant definitions

$$\delta_\omega = \sqrt{(\omega_x^2 \Delta y \Delta z + \omega_y^2 \Delta x \Delta z + \omega_z^2 \Delta x \Delta y)/|\omega|^2} \Longleftarrow \textbf{Chauvet et al. (2007)}$$

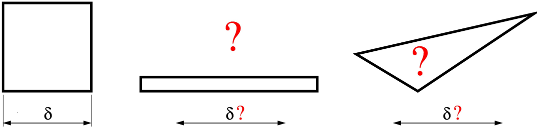
$$\tilde{\delta}_\omega = \frac{1}{\sqrt{3}} \max_{n,m=1,\dots,8} |l_n - l_m| \Longleftarrow \textbf{Mockett et al. (2015)}$$

$$\delta_{\mathrm{SLA}} = \tilde{\delta}_\omega F_{\mathrm{KH}}(VTM) \Longleftarrow \textbf{Shur et al. (2015)}$$

Building a new subgrid characteristic length for LES

Research question:

- Can we find a **simple and robust** definition of δ that minimizes the effect of **mesh anisotropies** on the performance of subgrid-scale models?



Building a new subgrid characteristic length for LES

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Starting point:

$$\underbrace{G \equiv \nabla \overline{u}}_{\text{physical space}} \qquad \underbrace{G_\delta \equiv G\Delta}_{\text{computational space}}$$

where for a Cartesian grid $\Delta \equiv \begin{bmatrix} \Delta x & & \\ & \Delta y & \\ & & \Delta z \end{bmatrix}$

Building a new subgrid characteristic length for LES

Idea: δ, appears in a natural way when we consider the leading term of the Taylor series expansion of the subgrid stress tensor,

$$\underbrace{\tau(\overline{u}) = \frac{\delta^2}{12} GG^T + \mathcal{O}(\delta^4)}_{\text{physical space}} \qquad \underbrace{\tau(\overline{u}) = \frac{1}{12} G_\delta G_\delta^T + \mathcal{O}(\delta^4)}_{\text{computational space}}$$

[6] F.X.Trias, A.Gorobets, M.Silvis, R.Verstappen, A.Oliva. *A new subgrid characteristic length for turbulence simulations on anisotropic grids*, **Phys.Fluids**, 26:115109, 2017.

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A **least-square minimization** leads to[6]

$$\delta_{\text{lsq}} = \sqrt{\frac{G_\delta G_\delta^T : GG^T}{GG^T : GG^T}}$$

[6] F.X.Trias, A.Gorobets, M.Silvis, R.Verstappen, A.Oliva. *A new subgrid characteristic length for turbulence simulations on anisotropic grids*, **Phys.Fluids**, 26:115109, 2017.

Building a new subgrid characteristic length for LES

Properties of new definition

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Building a new subgrid characteristic length for LES

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- Well-bounded: $\Delta x \leqslant \delta_{\text{lsq}} \leqslant \Delta z$ (assuming $\Delta x \leqslant \Delta y \leqslant \Delta z$)

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- Sensitive to flow orientation, *e.g.* for rotating flows ($G = \Omega$)

$$\delta_{\mathrm{lsq}} = \sqrt{\frac{\omega_x^2(\Delta y^2 + \Delta z^2) + \omega_y^2(\Delta x^2 + \Delta z^2) + \omega_z^2(\Delta x^2 + \Delta y^2)}{2|\omega|^2}}$$

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- Applicable to unstructured grid

Idea: $\dfrac{\partial \phi}{\partial x} \approx \dfrac{\phi_{i+1} - \phi_i}{\Delta x} \implies$ you can compute G; then, you can compute δ_{lsq}!

Building a new subgrid characteristic length for LES

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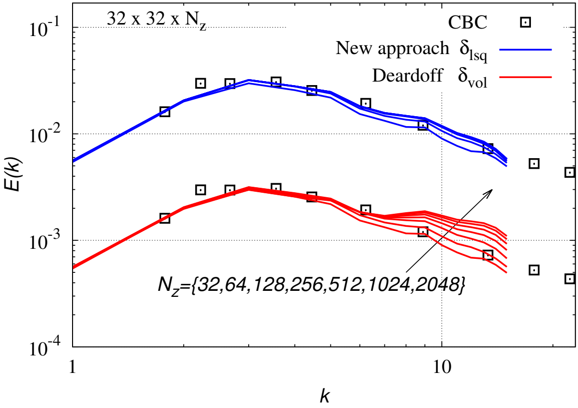
- Easy and cheap

Results for LES

Decaying isotropic turbulence

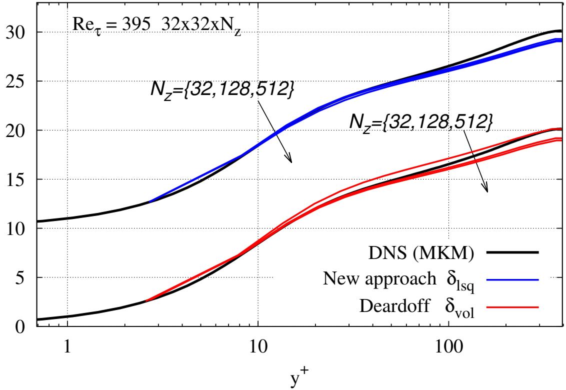
Comparison with classical Comte-Bellot & Corrsin (CBC) experiment



Results for LES

Turbulent channel flow

$Re_\tau = 395$ DNS Moser et al. LES $32 \times 32 \times N_z$



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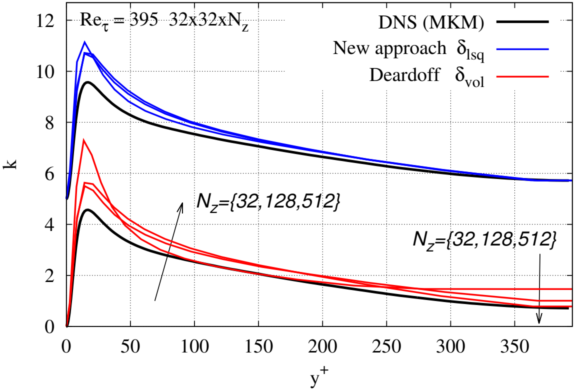
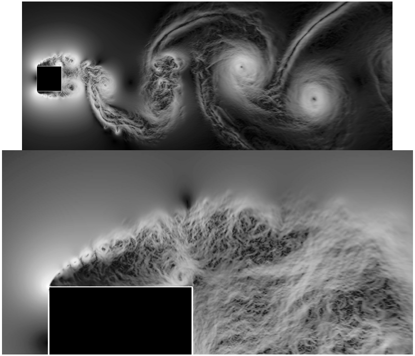


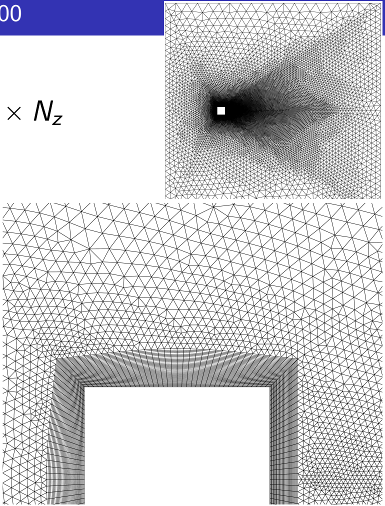
Results for LES

Turbulent flow around square cylinder at $Re = 22000$

DNS[7] 324M grid points

LES $19524 \times N_z$



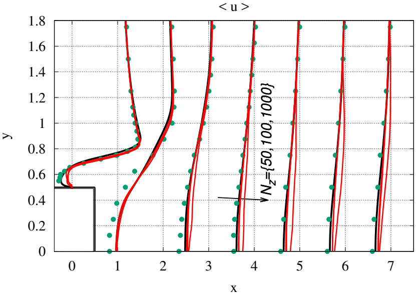


[7]F.X.Trias, A.Gorobets, A.Oliva. *Turbulent flow around a square cylinder at Reynolds number 22000: a DNS study*, **Computers&Fluids**, 123:87-98, 2015.

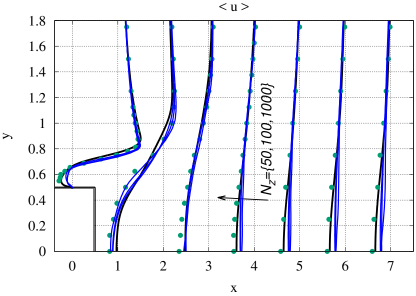
Results for LES

Turbulent flow around square cylinder at $Re = 22000$

LES[8] $19524 \times N_z$



Deardorff δ_{vol}



New approach δ_{lsq}

[8] F.X.Trias, D.Folch, A.Gorobets, A.Oliva. *Building proper invariants for eddy-viscosity subgrid-scale models*, **Physics of Fluids**, 27: 065103, 2015.

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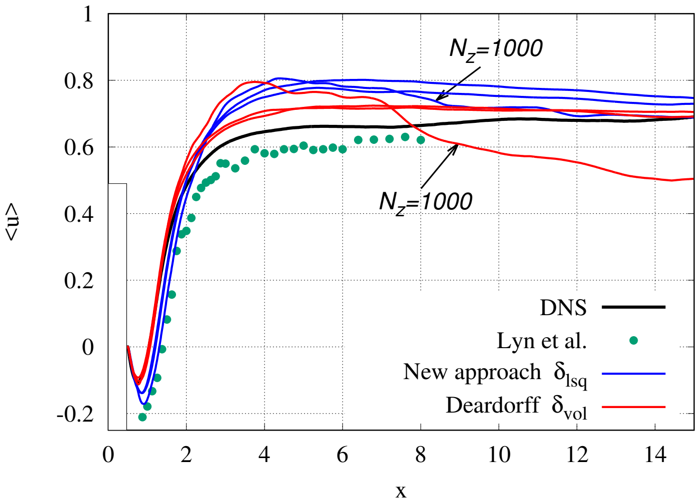

PHYSICS OF FLUIDS **29**, 115109 (2017)

A new subgrid characteristic length for turbulence simulations on anisotropic grids

F. X. Trias,[1,a)] A. Gorobets,[1,2,b)] M. H. Silvis,[3,c)] R. W. C. P. Verstappen,[3,d)] and A. Oliva[1,e)]
[1]*Heat and Mass Transfer Technological Center, Technical University of Catalonia, C/Colom 11, 08222 Terrassa, Spain*
[2]*Keldysh Institute of Applied Mathematics, 4A, Miusskaya Sq., Moscow 125047, Russia*
[3]*Johann Bernoulli Institute for Mathematics and Computer Science, University of Groningen, P.O. Box 407, 9700 AK Groningen, The Netherlands*

(Received 12 May 2017; accepted 6 November 2017; published online 29 November 2017)

Direct numerical simulations of the incompressible Navier-Stokes equations are not feasible yet for most practical turbulent flows. Therefore, dynamically less complex mathematical formulations are necessary for coarse-grained simulations. In this regard, eddy-viscosity models for Large-Eddy Simulation (LES) are probably the most popular example thereof. This type of models requires the calculation of a subgrid characteristic length which is usually associated with the local grid size. For isotropic grids, this is equal to the mesh step. However, for anisotropic or unstructured grids, such as the pancake-like meshes that are often used to resolve near-wall turbulence or shear layers, a consensus on defining the subgrid characteristic length has not been reached yet despite the fact that it can strongly affect the performance of LES models. In this context, a new definition of the subgrid characteristic length is presented in this work. This flow-dependent length scale is based on the turbulent, or subgrid stress, tensor and its representations on different grids. The simplicity and mathematical properties suggest that it can be a robust definition that minimizes the effects of mesh anisotropies on simulation results. The performance of the proposed subgrid characteristic length is successfully tested for decaying isotropic turbulence and a turbulent channel flow using artificially refined grids. Finally, a simple extension of the method for unstructured meshes is proposed and tested for a turbulent flow around a square cylinder. Comparisons with existing subgrid characteristic length scales show that the proposed definition is much more robust with respect to mesh anisotropies and has a great potential to be used in complex geometries where highly skewed (unstructured) meshes are present. *Published by AIP Publishing.* https://doi.org/10.1063/1.5012546

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$$\delta_{\mathrm{SLA}} = \tilde{\delta}_{\omega} F_{\mathrm{KH}}(VTM) \Longleftarrow \textbf{Shur et al. (2015)}$$

Subgrid length scales for DES

Is the new δ_{lsq} a good candidate?

New definition[9,10] (PoF'17; HRLM7 2018):

$$\delta_{\text{lsq}} = \sqrt{\frac{G_\delta G_\delta^T : GG^T}{GG^T : GG^T}}$$

Mockett *et al.* (HRLM5, 2015):

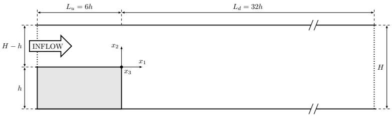
$$\tilde{\delta}_\omega = \frac{1}{\sqrt{3}} \max_{n,m=1,\dots,8} |I_n - I_m|$$

[9] F.X.Trias, A.Gorobets, M.Silvis, R.Verstappen, A.Oliva. *A new subgrid characteristic length for turbulence simulations on anisotropic grids*, **Phys.Fluids**, 26:115109, 2017.

[10] A.Pont, F.X.Trias, A.Revell, A.Oliva. *Assessment and comparison of a recent kinematic sensitive subgrid length scale in Hybrid RANS-LES*. **HRLM7**, Berlin, 2018.

Test case: backward facing step

DNS (A.Pont, F.X.Trias, A.Gorobets, A.Oliva, submitted to JFM)



- $ER = H/(H-h) = 2$
- $Re_h \sim 13700$, $Re_\tau = 395$
- Geom: $(6h + 32h) \times (h + h) \times 2h$
- Mesh DNS: $1510 \times 302 \times 360 \approx$ **164M**
- Mesh DES: $332 \times 86 \times 60 \approx$ **1.5M**

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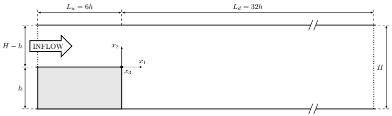

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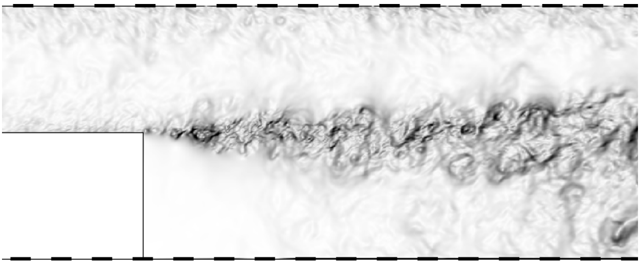

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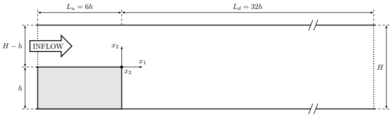

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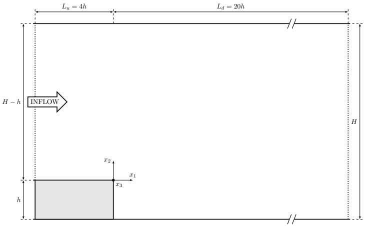
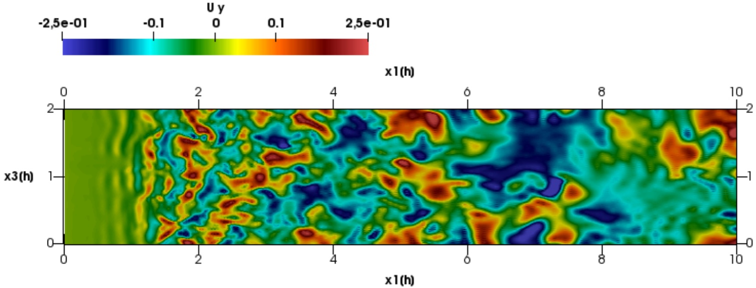
Experimental study (Vogel and Eaton, 1985)



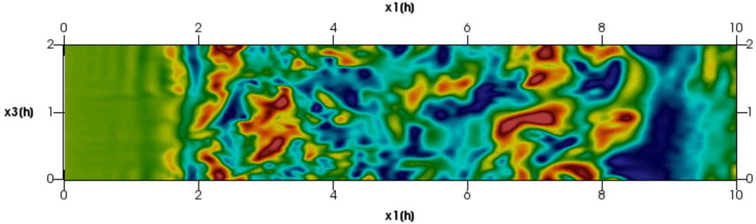
- $ER = H/(H-h) = 5/4$
- $Re_h = 28000$, $Re_\tau = 2500$
- Geom: $(4h + 20h) \times (h + 4h) \times 2h$
- Mesh DES:$300 \times 79 \times 60 \approx$ **1.28M**

BFS (Vogel and Eaton, 1985): $u_2' = u_2 - \langle u_2 \rangle$

$\delta_{\rm lsq}$



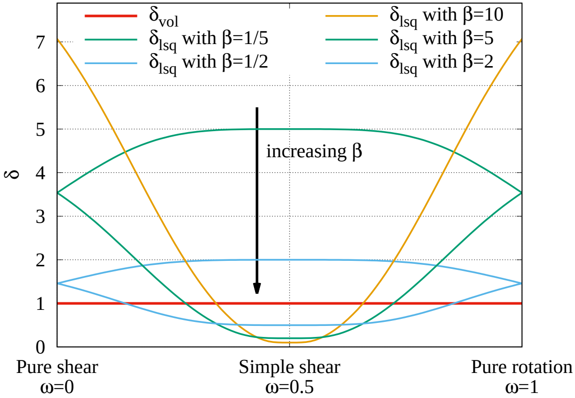
$\tilde{\delta}_\omega$



Properties of new definition in the shear layer

Simple 2D flow analysis

$$\Delta = \begin{pmatrix} \beta & 0 \\ 0 & \beta^{-1} \end{pmatrix} \qquad G = \begin{pmatrix} 0 & 1 \\ 1-2\omega & 0 \end{pmatrix}$$



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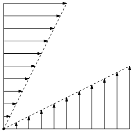
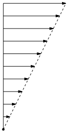
Canonical flow configurations:



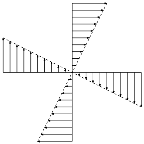
$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Pure Shear ($\omega = 0$)



$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

Simple Shear (ω=0.5)



$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

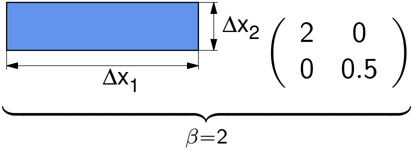
Pure Rotation (ω=1)

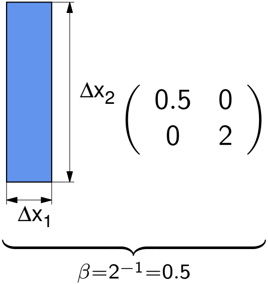
Properties of new definition in the shear layer

Simple 2D flow analysis

$$\Delta = \begin{pmatrix} \beta & 0 \\ 0 & \beta^{-1} \end{pmatrix} \qquad G = \begin{pmatrix} 0 & 1 \\ 1-2\omega & 0 \end{pmatrix}$$

Examples of control volumes:





Properties of new definition in the shear layer

Simple 2D flow analysis: $\tilde{\delta}_\omega$ vs δ_{lsq}

$$\Delta = \begin{pmatrix} \beta & 0 \\ 0 & \beta^{-1} \end{pmatrix} \qquad G = \begin{pmatrix} 0 & 1 \\ 1 - 2\omega & 0 \end{pmatrix}$$

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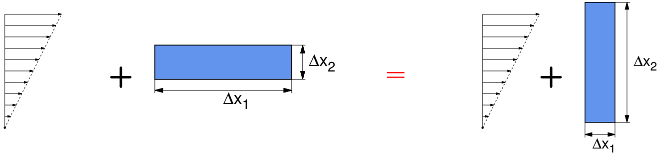

⚠ Unsensitive to mesh rotation for simple shear flow ($\omega = 0.5$)

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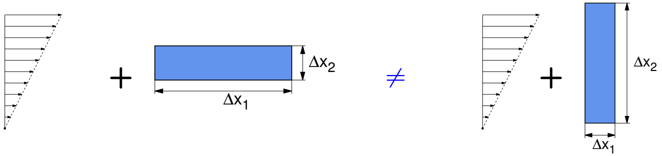

For $\omega = 0.5$ (simple shear) $\implies$ $\delta_{\mathrm{lsq}} = \beta^{-1} (= \Delta x_2)$

Improving LES models for buoyancy-driven flows

$$\partial_t \overline{u} + (\overline{u} \cdot \nabla)\overline{u} = \nu \nabla^2 \overline{u} - \nabla \overline{p} \qquad - \nabla \cdot \tau(\overline{u}) \;\; ; \qquad \nabla \cdot \overline{u} = 0$$

eddy-viscosity $\longrightarrow$ $\tau\;(\overline{u}) = -2\nu_t S(\overline{u})$

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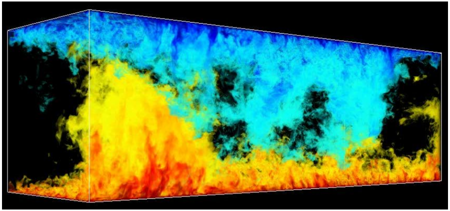

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⚠ But first we need to answer the following **research question**:

- Are **eddy-viscosity models** for momentum able to provide satisfactory results for turbulent Rayleigh-Bénard convection?

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⚠ But first we need to answer the following **research question**:

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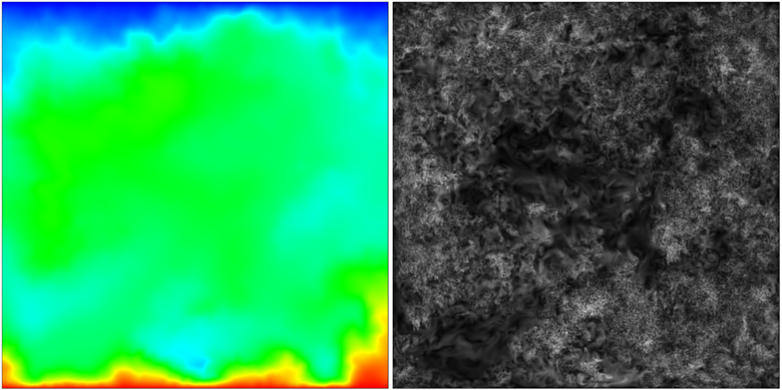
Idea: let's do an LES for momentum and a DNS for temperature!

DNS at very low Pr number

Why? scale separation scales with $Pr^{0.5}$

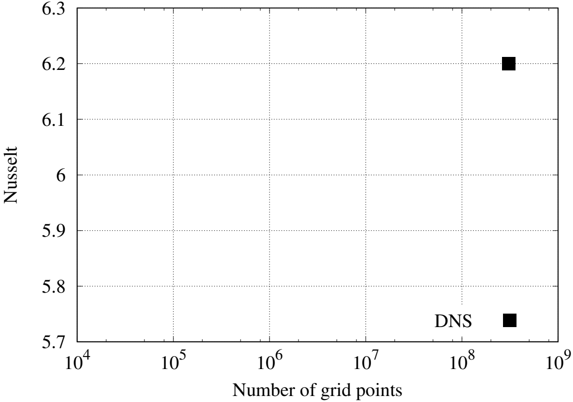
DNS at very low *Pr* number

Why? scale separation scales with $Pr^{0.5}$ (≈ 0.07 is our case)



DNS of a RB at $Ra = 7.14 \times 10^6$ and $Pr = 0.005$ (liquid sodium)

LES[11] results at very low *Pr* number



[11] F.X.Trias, D.Folch, A.Gorobets, A.Oliva. *Building proper invariants for eddy-viscosity subgrid-scale models*, **Physics of Fluids**, 27: 065103, 2015.

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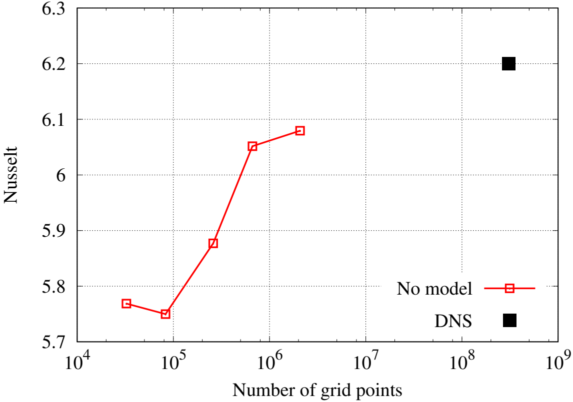

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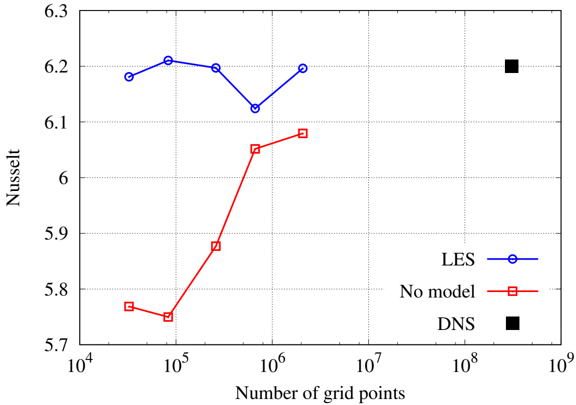

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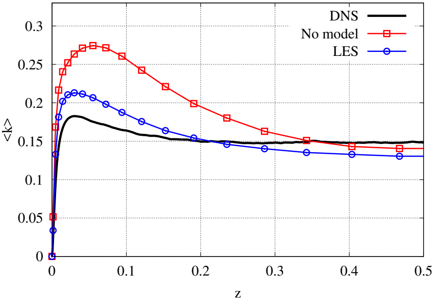
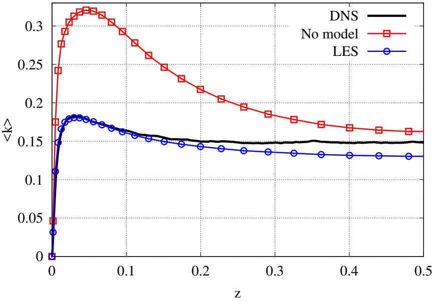
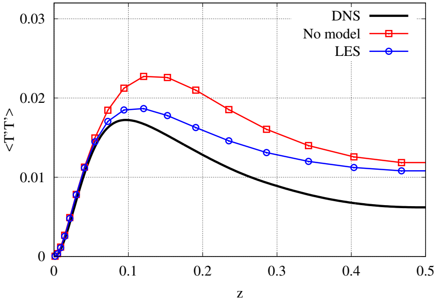


$64 \times 32 \times 32$



$96 \times 52 \times 52$

LES results at very low *Pr* number



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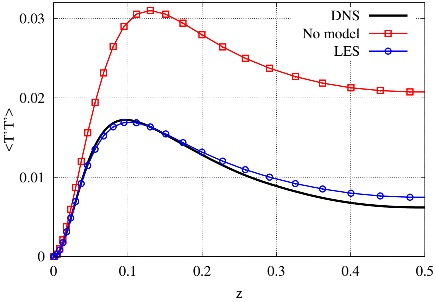

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Concluding remarks

- A new definition for δ has been proposed

$$\delta_{\mathrm{lsq}} = \sqrt{\frac{G_\delta G_\delta^T : GG^T}{GG^T : GG^T}}$$

- LES tests: HIT, channel flow, square cylinder (unstructured) ✓
- DES tests: backward facing step, turbulent jet (not shown here) ✓
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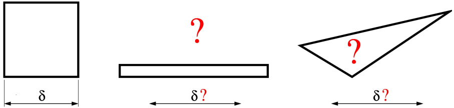

Takeaway message:

- Definition of δ can have a big effect on simulation results

Thank you for your attention