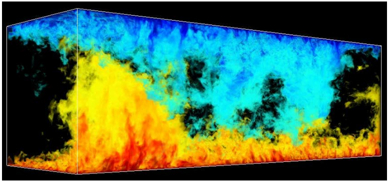
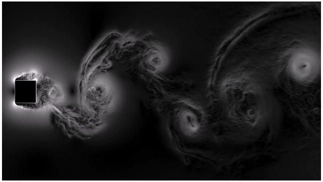
Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA
JOHANNES KEPLER UNIVERSITY LINZ

Proper SGS heat flux models for LES

F.Xavier Trias[1], Daniel Santos[1], Firas Dabbagh[2], Andrey Gorobets[3], Assensi Oliva[1]

[1]Heat and Mass Transfer Technological Center, Technical University of Catalonia
[2]Christian-Doppler Laboratory for Multi-scale Modelling of Multiphase Processes, Johannes Kepler University, Linz, Austria
[3]Keldysh Institute of Applied Mathematics of RAS, Russia





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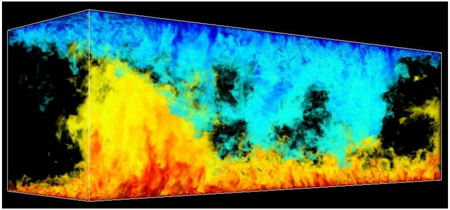
Contents

Motivation

Research question #1:

- 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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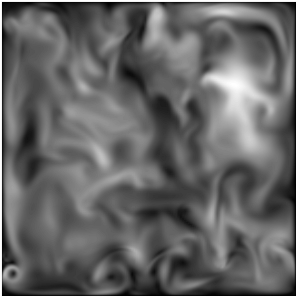
Air-filled RB: $Pr = 0.7$

$Ra = 10^8$



[2]F.Dabbagh, F.X.Trias, A.Gorobets, A.Oliva. *Flow topology dynamics in a 3D phase space for turbulent Rayleigh-Bénard convection*, **Phys.Rev.Fluids**, 5:024603, 2020.

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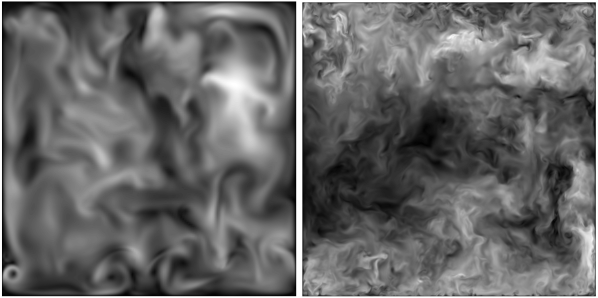

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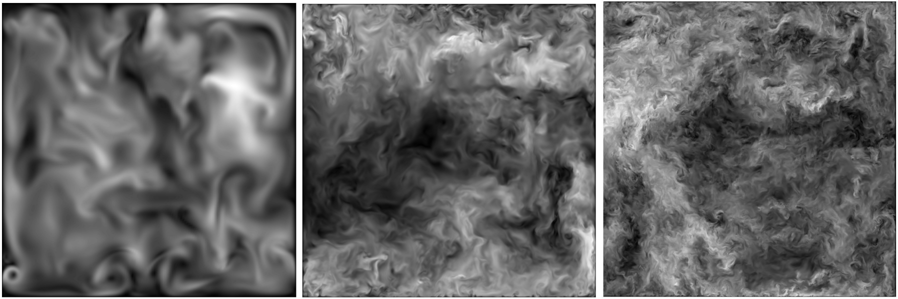

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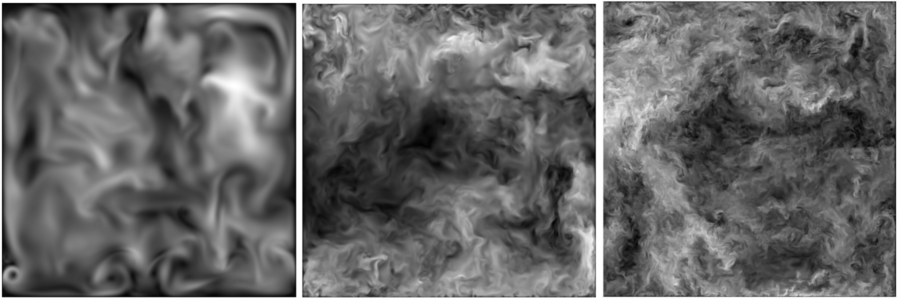

$208 \times 208 \times 400$ **17.5M** | $768 \times 768 \times 1024$ **607M** | $1662 \times 1662 \times 2048$ **5600M**

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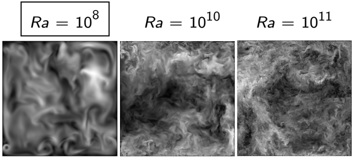

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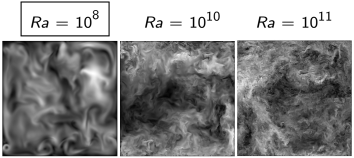
DNS: $208 \times 208 \times 400$

LES: $80 \times 80 \times 120$



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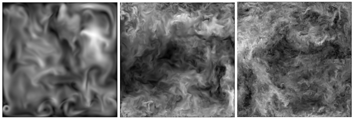

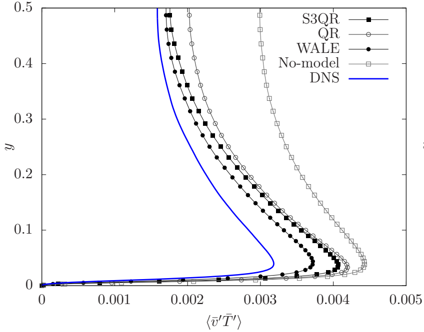

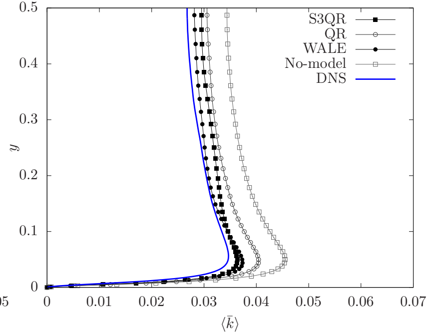

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DNS: $208 \times 208 \times 400$

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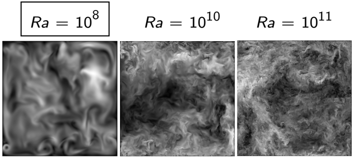
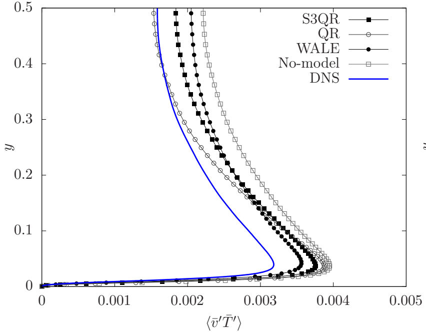
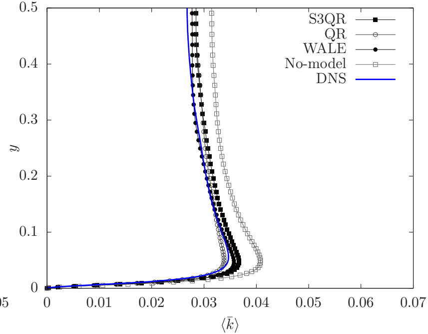


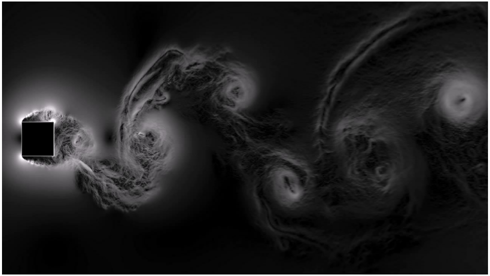


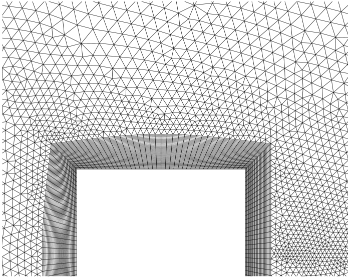


Motivation

Research question #2:

- Can we construct numerical discretizations of the Navier-Stokes equations suitable for **complex geometries**, such that the **symmetry properties** are exactly preserved?



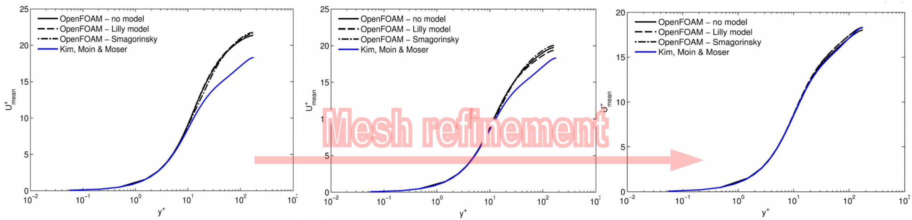


DNS[3] of the turbulent flow around a square cylinder at $Re = 22000$

[3] 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.

Motivation

OpenFOAM® LES[4] results of a turbulent channel for at $Re_\tau = 180$



$13 \times 76 \times 20$	$19 \times 78 \times 28$	$38 \times 78 \times 57$
$\Delta x^+ = 90, \Delta y^+_{wall} = 0.5, \Delta z^+ = 30$	$\Delta x^+ = 60, \Delta y^+_{wall} = 0.5, \Delta z^+ = 20$	$\Delta x^+ = 30, \Delta y^+_{wall} = 0.5, \Delta z^+ = 10$

[4] E.M.J.Komen, L.H.Camilo, A.Shams, B.J.Geurts, B.Koren. *A quantification method for numerical dissipation in quasi-DNS and under-resolved DNS, and effects of numerical dissipation in quasi-DNS and under-resolved DNS of turbulent channel flows*, **Journal of Computational Physics**, 345, 565-595, 2017.

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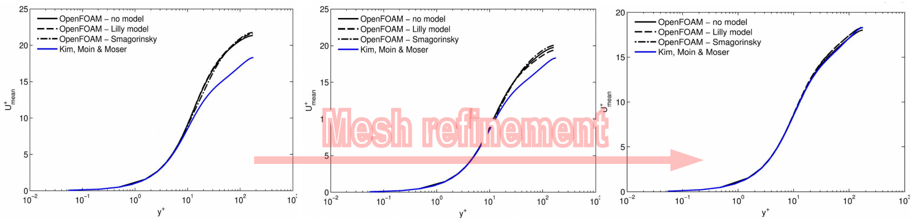

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- Are LES results a merit of the SGS model?

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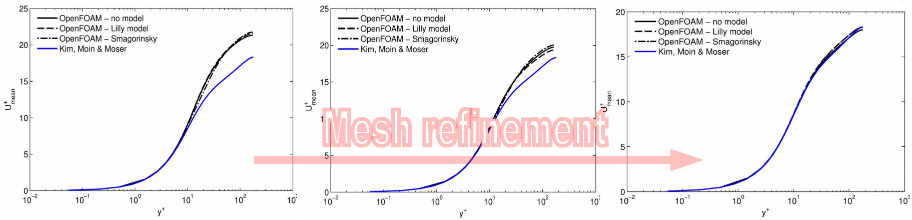

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- Are LES results a merit of the SGS model? Apparently **NOT**!!! ✗

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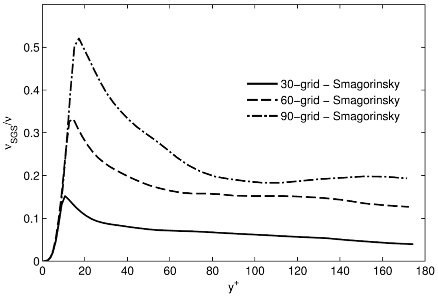

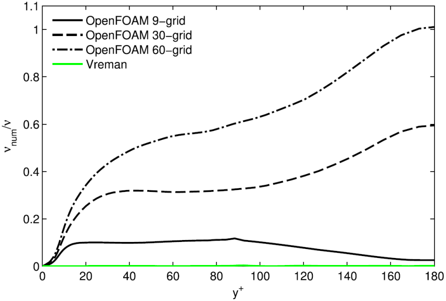

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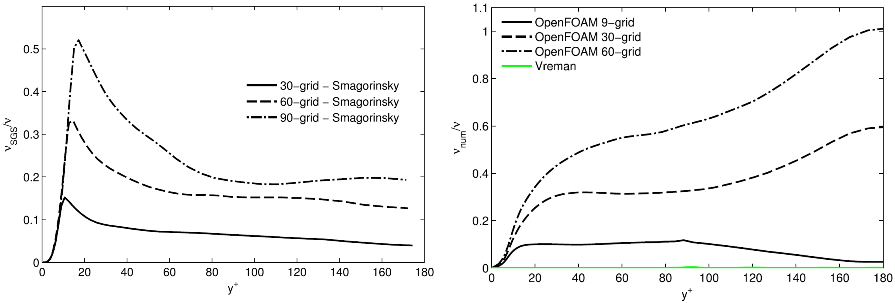

$$\nu_{SGS} < \nu_{num} \neq 0$$

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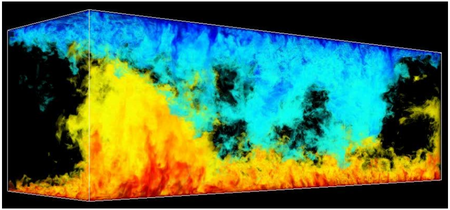

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How to model the subgrid heat flux in LES?

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

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

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$$Pr_t?$$

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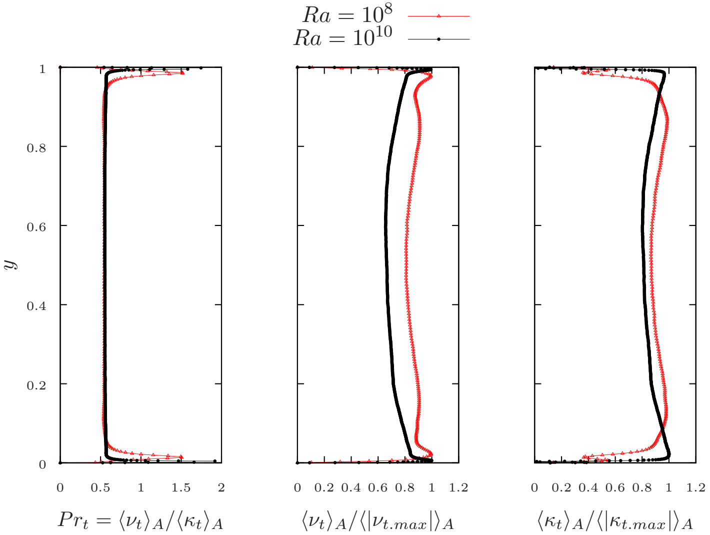

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$$G \equiv \nabla \overline{\boldsymbol{u}} \qquad\qquad \boldsymbol{q} = -\frac{\delta^2}{12} G \nabla \overline{T} + \mathcal{O}(\delta^4)$$

A priori alignment trends[6]

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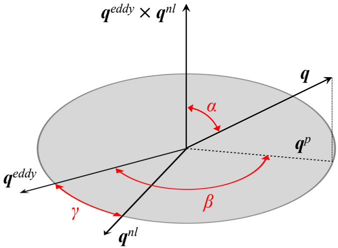

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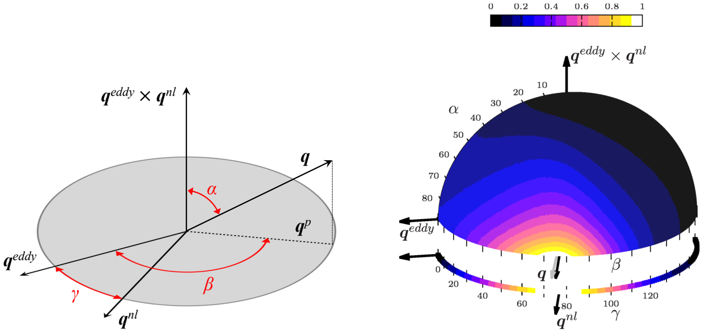

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[7] S.Peng and L.Davidson. **Int.J.Heat Mass Transfer**, 45:1393-1405, 2002.

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gradient model $\longrightarrow \quad \boldsymbol{q} \approx -\frac{\delta^2}{12} G \nabla \overline{T} \qquad (\equiv \boldsymbol{q}^{nl})$

Peng&Davidson[7] $\longrightarrow \quad \boldsymbol{q} \approx -\frac{\delta^2}{12} S \nabla \overline{T} \qquad (\equiv \boldsymbol{q}^{PD})$

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A priori alignment trends

$$\boldsymbol{q}^{nl} \equiv -\frac{\delta^2}{12} G \nabla \overline{T}$$

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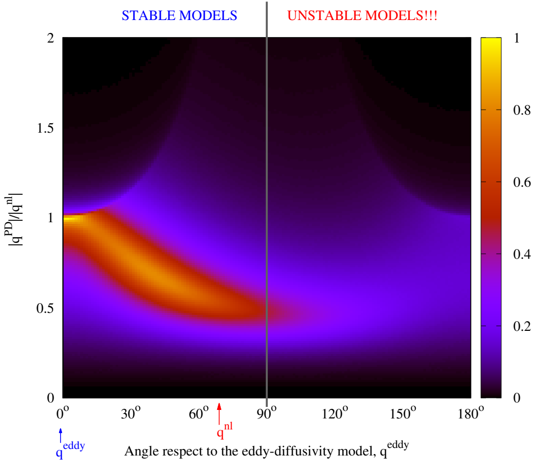

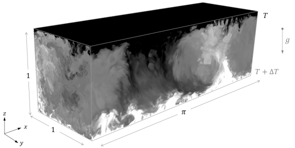

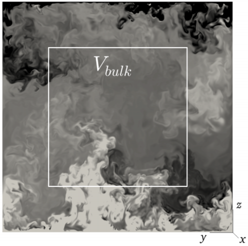

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[8] B.J.Daly and F.H.Harlow. **Physics of Fluids**, 13:2634, 1970.

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Daly&Harlow[8] $\longrightarrow$ $\boldsymbol{q} \approx -\mathcal{T}_{SGS} \dfrac{\delta^2}{12} G G^T \nabla \overline{T}$ $\quad (\equiv \boldsymbol{q}^{DH})$

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$$\mathcal{T}_{SGS} = 1/|S|$$

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A priori alignment trends

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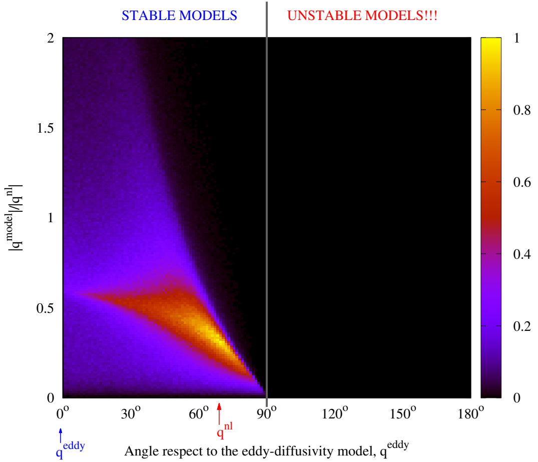

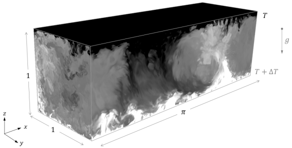

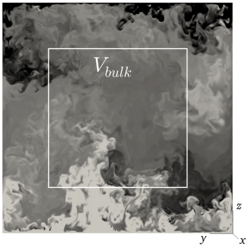

What about near-wall scaling?

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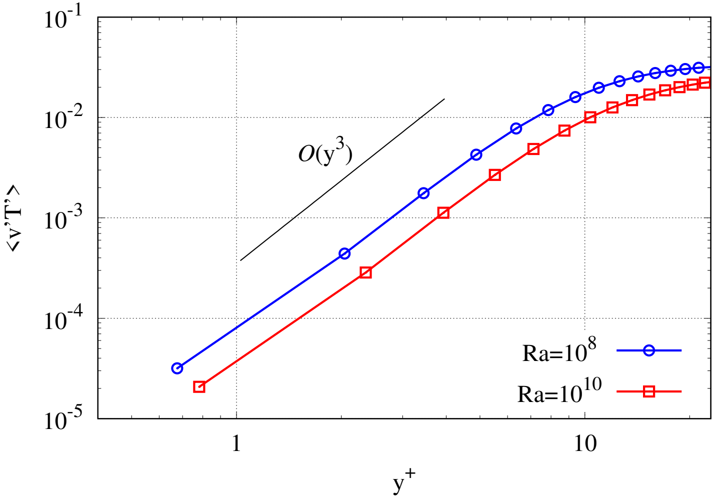
$\Longrightarrow$ Answer: it should be $\mathcal{O}(y^3)$



Near-wall scaling for DH model?

$$\boldsymbol{q}^{DH} \equiv -\mathcal{T}_{SGS} \frac{\delta^2}{12} GG^T \nabla \overline{T} \, ; \qquad \mathcal{T}_{SGS} = 1/|S|$$

Near-wall scaling for DH model? $\Longrightarrow$ Answer: it is $\mathcal{O}(y^1)$ instead of $\mathcal{O}(y^3)$

$$\boxed{\boldsymbol{q}^{DH} \equiv -\mathcal{T}_{SGS}\frac{\delta^2}{12}GG^T\nabla\overline{T}\;; \qquad \mathcal{T}_{SGS} = 1/|S|}$$

$$u = ay + \mathcal{O}(y^2);\quad v = by^2 + \mathcal{O}(y^3);\quad w = cy + \mathcal{O}(y^2);\quad T = dy + \mathcal{O}(y^2)$$

$$G = \begin{pmatrix} y & 1 & y \\ y^2 & y & y^2 \\ y & 1 & y \end{pmatrix};\ \nabla\overline{T} = \begin{pmatrix} y \\ 1 \\ y \end{pmatrix} \Longrightarrow \boxed{GG^T\nabla\overline{T} = \begin{pmatrix} y \\ y^2 \\ y \end{pmatrix} = \mathcal{O}(y^1)}$$

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$$\boxed{\mathcal{T}_{SGS} = 1/|S| = \mathcal{O}(y^0)}$$

Idea: build a $\mathcal{T}_{SGS}$ with the proper $\mathcal{O}(y^2)$ scaling!!!

Building proper models for the subgrid heat flux[9]

Let us consider models that are based on the invariants of the tensor GG^T

$$\boldsymbol{q} \approx -C_M \left(P_{GG^T}^{p} Q_{GG^T}^{q} R_{GG^T}^{r} \right) \frac{\delta^2}{12} GG^T \nabla \overline{T} \qquad (\equiv \boldsymbol{q}^{S2})$$

[9] F.X.Trias, F.Dabbagh, A.Gorobets, C.Oliet. *On a proper tensor-diffusivity model for LES of buoyancy-driven turbulence*, **Flow Turbul Combust**, 105:393-414, 2020.

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	P_{GG^T}	Q_{GG^T}	R_{GG^T}
Formula	$2(Q_\Omega - Q_S)$	$V^2 + Q_G^2$	R_G^2
Wall-behavior	$\mathcal{O}(y^0)$	$\mathcal{O}(y^2)$	$\mathcal{O}(y^6)$
Units	$[T^{-2}]$	$[T^{-4}]$	$[T^{-6}]$

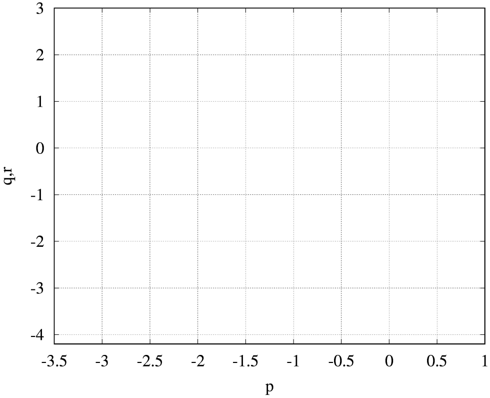
$$-6r - 4q - 2p = 1 \;\; [T]; \qquad 6r + 2q = s,$$

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

[9] F.X.Trias, F.Dabbagh, A.Gorobets, C.Oliet. *On a proper tensor-diffusivity model for LES of buoyancy-driven turbulence*, **Flow Turbul Combust**, 105:393-414, 2020.

Building proper models for the subgrid heat flux[9]

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



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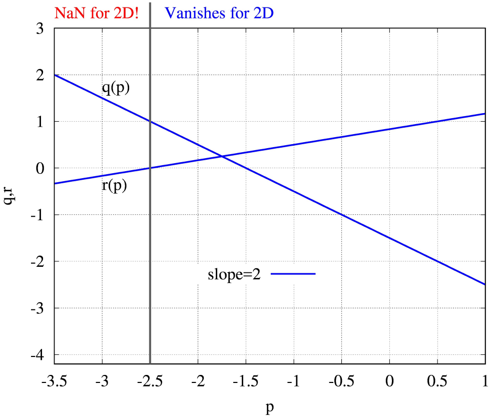

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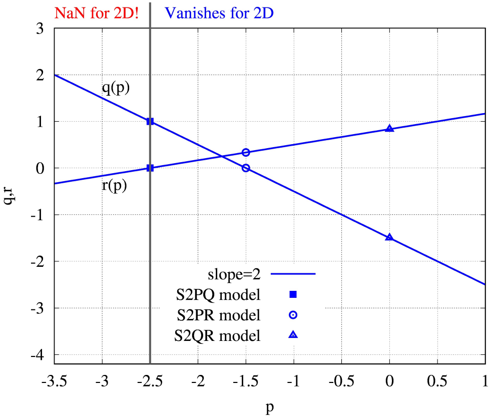

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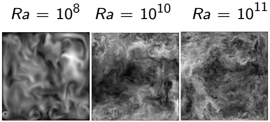
A priori analysis in the bulk

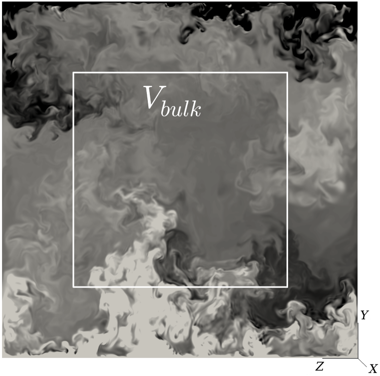
Estimation of the model constant, C_{s2pqr}

Playing with exponent p...

$$\boldsymbol{q}^{S2PQR} \approx -C_{s2pqr} \left(P^{p}_{GG^T} Q^{-(p+3/2)}_{GG^T} R^{(2p+5)/6}_{GG^T} \right) \frac{\delta^2}{12} GG^T \nabla \overline{T}$$



$$\frac{< |\boldsymbol{q}^{S2PQR}| >_{bulk}}{< |\boldsymbol{q}| >_{bulk}} = 1 \longrightarrow C_{s2pqr}$$



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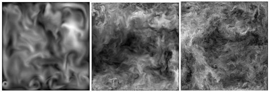
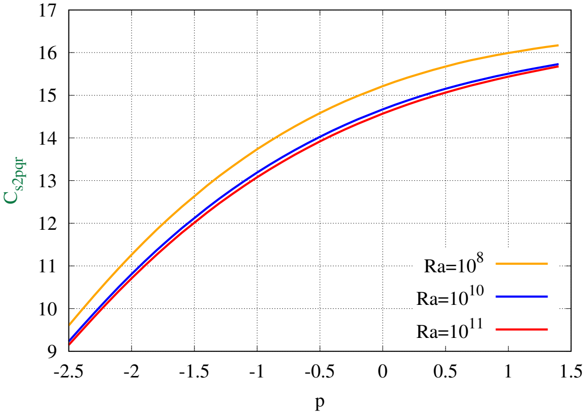
$Ra = 10^8$ $Ra = 10^{10}$ $Ra = 10^{11}$





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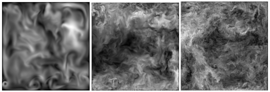

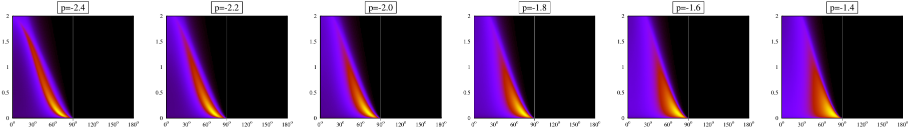

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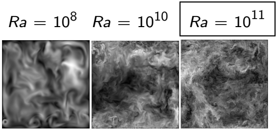

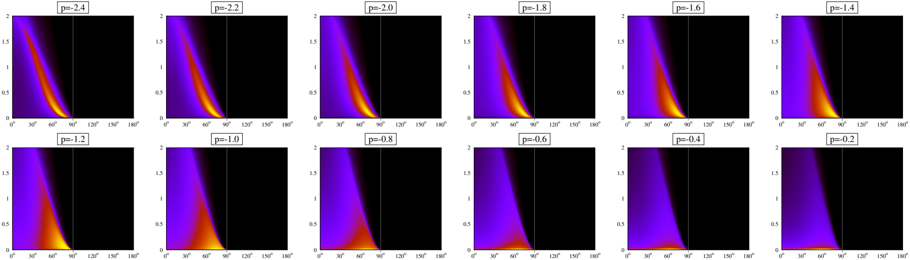

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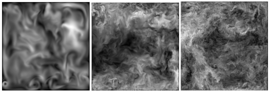
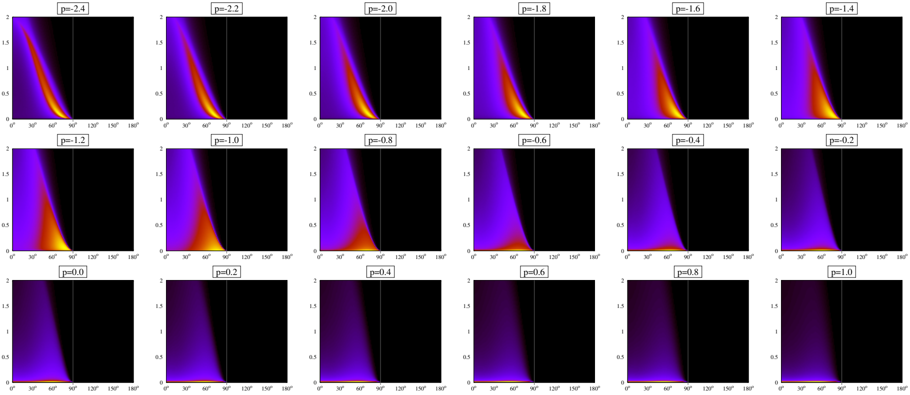
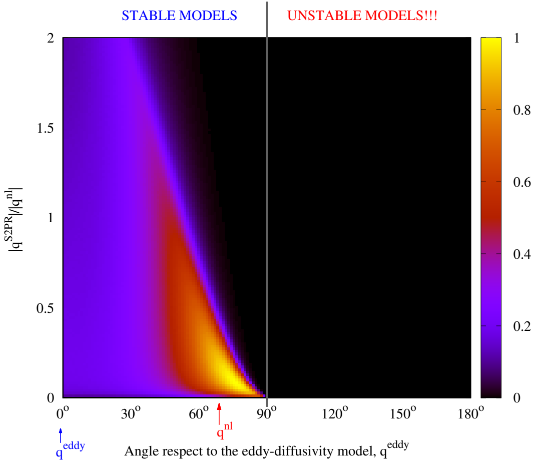


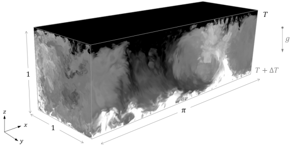


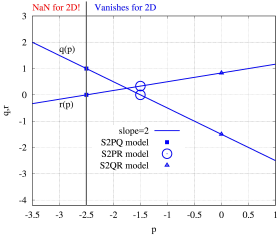
A priori alignment trends of S2PR in the bulk

$$\boldsymbol{q}^{nl} \equiv -\frac{\delta^2}{12} G \nabla \overline{T}$$

$$\boldsymbol{q}^{s2PR} \equiv -C_{s2pr} P_{GG^T}^{-3/2} R_{GG^T}^{1/3} \frac{\delta^2}{12} GG^T \nabla \overline{T}$$



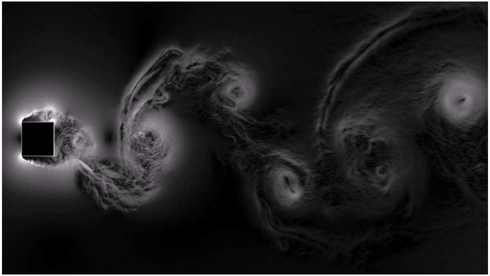


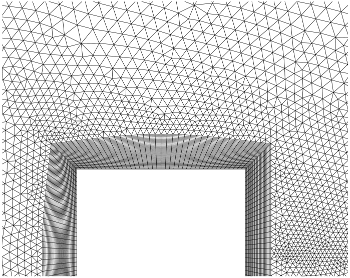


Motivation

Research question #2:

- Can we construct numerical discretizations of the Navier-Stokes equations suitable for **complex geometries**, such that the **symmetry properties** are exactly preserved?





DNS[3] of the turbulent flow around a square cylinder at $Re = 22000$

[3] 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.

Symmetry-preserving discretization

Continuous

$$\frac{\partial \boldsymbol{u}}{\partial t} + C(\boldsymbol{u}, \boldsymbol{u}) = \nu \nabla^2 \boldsymbol{u} - \nabla p$$

$$\nabla \cdot \boldsymbol{u} = 0$$

Symmetry-preserving discretization

Continuous	Discrete
$\frac{\partial \boldsymbol{u}}{\partial t} + C(\boldsymbol{u}, \boldsymbol{u}) = \nu \nabla^2 \boldsymbol{u} - \nabla p$	$\Omega \frac{d\boldsymbol{u}_h}{dt} + \mathsf{C}(\boldsymbol{u}_h)\,\boldsymbol{u}_h = \mathsf{D}\boldsymbol{u}_h - \mathsf{G}\boldsymbol{p}_h$
$\nabla \cdot \boldsymbol{u} = 0$	$\mathsf{M}\boldsymbol{u}_h = \boldsymbol{0}_h$

Symmetry-preserving discretization

Continuous	Discrete
$\frac{\partial \boldsymbol{u}}{\partial t} + C(\boldsymbol{u}, \boldsymbol{u}) = \nu \nabla^2 \boldsymbol{u} - \nabla p$	$\Omega \frac{d \boldsymbol{u}_h}{dt} + \mathsf{C}(\boldsymbol{u}_h) \boldsymbol{u}_h = \mathsf{D} \boldsymbol{u}_h - \mathsf{G} \boldsymbol{p}_h$
$\nabla \cdot \boldsymbol{u} = 0$	$\mathsf{M} \boldsymbol{u}_h = \boldsymbol{0}_h$
$\langle \boldsymbol{a}, \boldsymbol{b} \rangle = \int_\Omega \boldsymbol{a} \boldsymbol{b} d\Omega$	$\langle \boldsymbol{a}_h, \boldsymbol{b}_h \rangle_h = \boldsymbol{a}_h^T \Omega \boldsymbol{b}_h$

Symmetry-preserving discretization

Continuous	Discrete
$$\frac{\partial \boldsymbol{u}}{\partial t} + C(\boldsymbol{u}, \boldsymbol{u}) = \nu \nabla^2 \boldsymbol{u} - \nabla p$$ $$\nabla \cdot \boldsymbol{u} = 0$$	$$\Omega \frac{d\boldsymbol{u}_h}{dt} + \mathsf{C}(\boldsymbol{u}_h)\boldsymbol{u}_h = \mathsf{D}\boldsymbol{u}_h - \mathsf{G}\boldsymbol{p}_h$$ $$\mathsf{M}\boldsymbol{u}_h = \boldsymbol{0}_h$$
$$\langle \boldsymbol{a}, \boldsymbol{b} \rangle = \int_\Omega \boldsymbol{a}\boldsymbol{b} d\Omega$$	$$\langle \boldsymbol{a}_h, \boldsymbol{b}_h \rangle_h = \boldsymbol{a}_h^T \Omega \boldsymbol{b}_h$$
$$\langle C(\boldsymbol{u}, \varphi_1), \varphi_2 \rangle = -\langle C(\boldsymbol{u}, \varphi_2), \varphi_1 \rangle$$	$$\mathsf{C}(\boldsymbol{u}_h) = -\mathsf{C}^T(\boldsymbol{u}_h)$$

Symmetry-preserving discretization

Continuous	Discrete
$\frac{\partial \boldsymbol{u}}{\partial t} + C(\boldsymbol{u}, \boldsymbol{u}) = \nu \nabla^2 \boldsymbol{u} - \nabla p$ $\nabla \cdot \boldsymbol{u} = 0$	$\Omega \frac{d\boldsymbol{u}_h}{dt} + \mathsf{C}(\boldsymbol{u}_h)\boldsymbol{u}_h = \mathsf{D}\boldsymbol{u}_h - \mathsf{G}\boldsymbol{p}_h$ $\mathsf{M}\boldsymbol{u}_h = \boldsymbol{0}_h$
$\langle \boldsymbol{a}, \boldsymbol{b} \rangle = \int_\Omega \boldsymbol{a}\boldsymbol{b} d\Omega$	$\langle \boldsymbol{a}_h, \boldsymbol{b}_h \rangle_h = \boldsymbol{a}_h^T \Omega \boldsymbol{b}_h$
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Symmetry-preserving discretization

Continuous	Discrete
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Why collocated arrangements are so popular?

- STAR-CCM+
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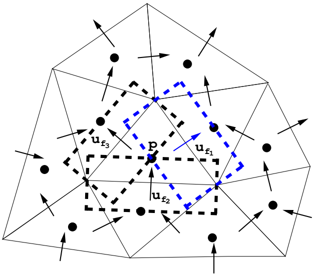
In staggered meshes

- p-$\boldsymbol{u}_s$ coupling is naturally solved ✓
- $\mathsf{C}(\boldsymbol{u}_s)$ and D difficult to discretize ✗



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In collocated meshes

- p-$\boldsymbol{u}_c$ coupling is cumbersome ✗
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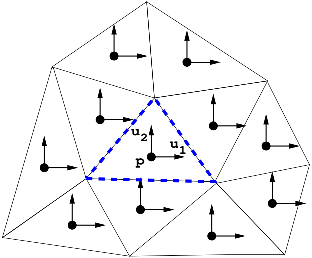
- Cheaper, less memory,... ✓



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Everything is easy except the pressure-velocity coupling...

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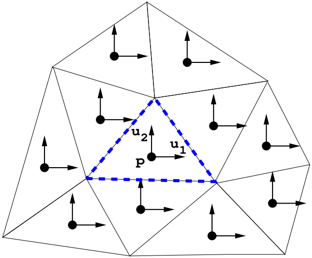

Pressure-velocity coupling on collocated grids

A vicious circle that cannot be broken...

In summary[10]:

- Mass: $M\Gamma_{c\rightarrow s}\boldsymbol{u}_c = M\Gamma_{c\rightarrow s}\boldsymbol{u}_c - \mathsf{L}_c\mathsf{L}^{-1} M\Gamma_{c\rightarrow s}\boldsymbol{u}_c \approx \mathbf{0}_c$ ✗
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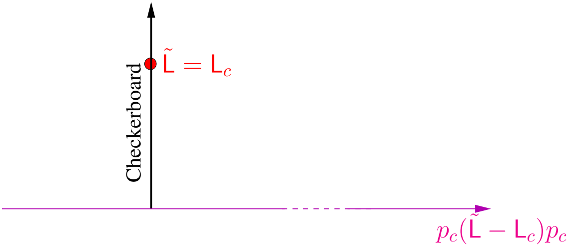

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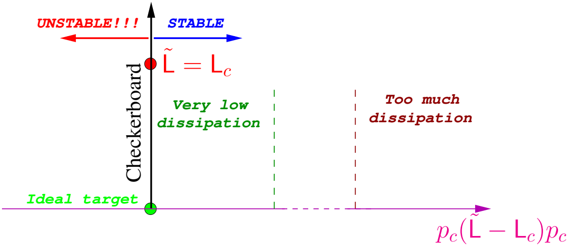

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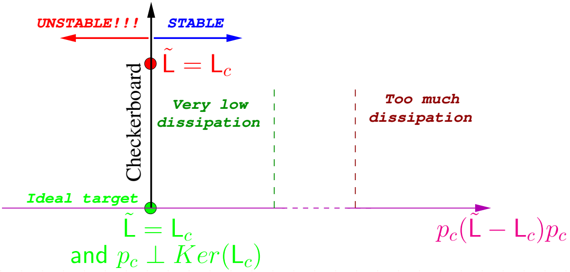

[10] Shashank, J.Larsson, G.Iaccarino. *A co-located incompressible Navier-Stokes solver with exact mass, momentum and kinetic energy conservation in the inviscid limit*, **Journal of Computational Physics**, 229: 4425-4430,2010.

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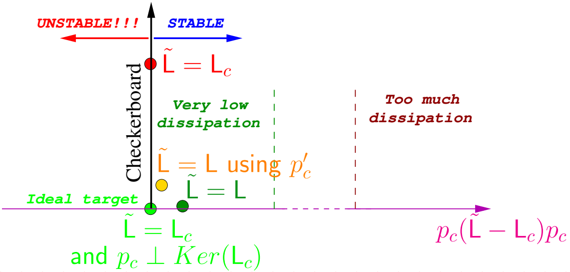

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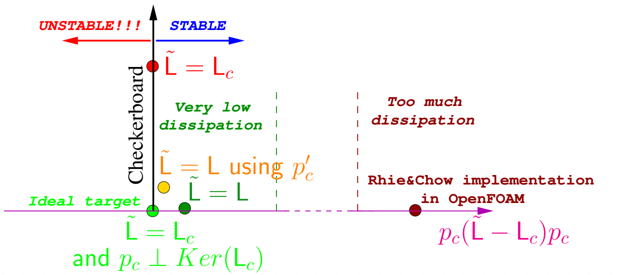

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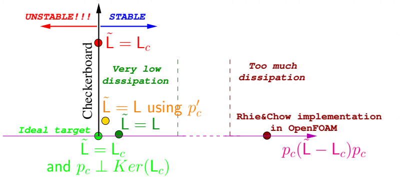

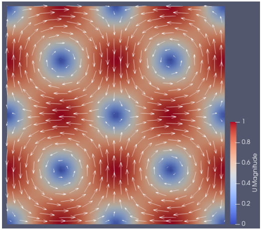

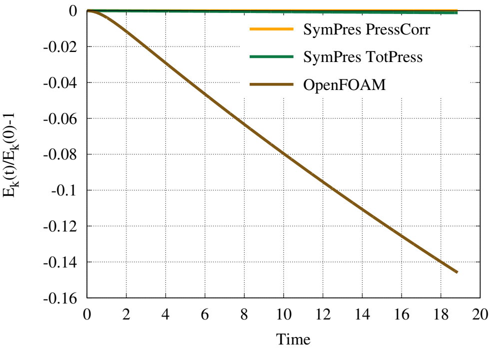

Results for an inviscid Taylor-Green vortex[11]

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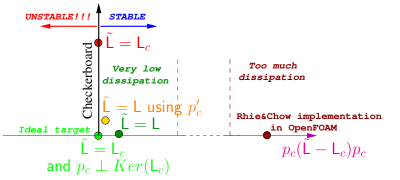

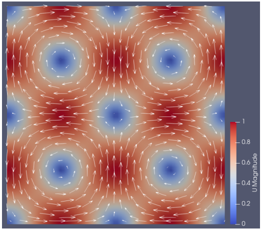

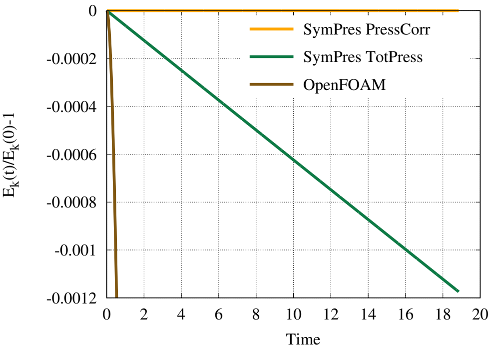

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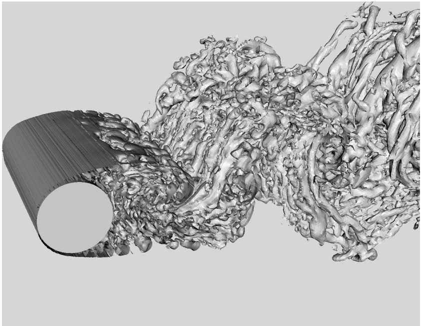
Pressure-velocity coupling on collocated grids

Examples of simulations

Despite these inherent limitations, symmetry-preserving collocated formulation has been successfully used for DNS/LES simulations[12]:



[12] R.Borrell, O.Lehmkuhl, F.X.Trias, A.Oliva. *Parallel Direct Poisson solver for discretizations with one Fourier diagonalizable direction*. **Journal of Computational Physics**, 230:4723-4741, 2011.

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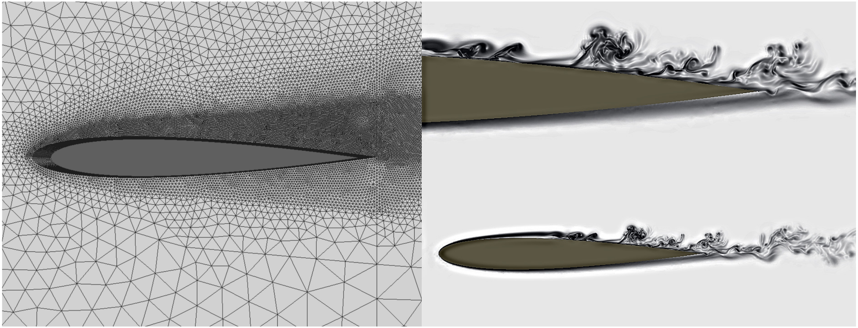

[12] F.X.Trias and O.Lehmkuhl. *A self-adaptive strategy for the time-integration of Navier-Stokes equations*. **Numerical Heat Transfer, part B**, 60(2):116-134, 2011.

Concluding remarks

- A new tensor-diffusivity model has been proposed

$$\boldsymbol{q}^{s2PR} \equiv -C_{s2pr} P_{GG^T}^{-3/2} R_{GG^T}^{1/3} \frac{\delta^2}{12} GG^T \nabla \overline{T}$$

- Locally defined, unconditionally stable and vanishes for 2D flows ✓
- Good *a priori* alignment trends and proper near-wall scaling ✓

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- *A posteriori* tests using $\boldsymbol{q}^{s2PR}$ for RB

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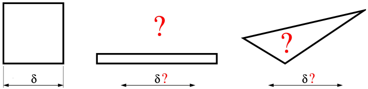

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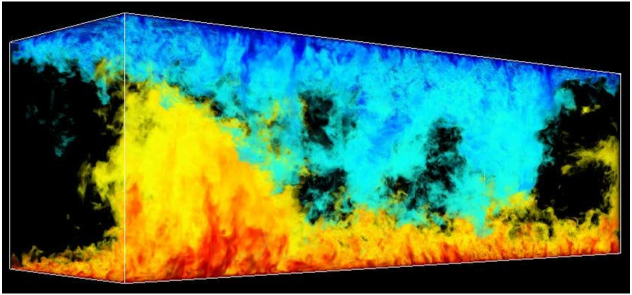
Thank you for your ~~virtual~~ hybrid attendance



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for Research & Innovation

Clean Sky 2
JOINT UNDERTAKING

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