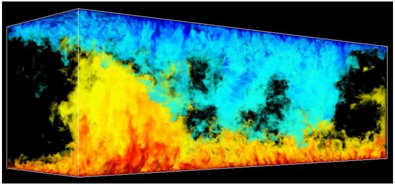
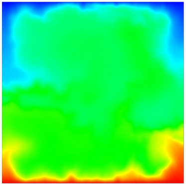
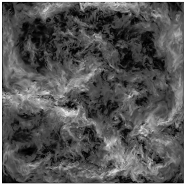
Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

DNS and LES of buoyancy-driven turbulence at high Rayleigh numbers

F.Xavier Trias[1], X.Álvarez-Farré[1], Daniel Santos[1], Andrey Gorobets[2], Assensi Oliva[1]

[1]Heat and Mass Transfer Technological Center, Technical University of Catalonia
[2]Keldysh Institute of Applied Mathematics of RAS, Russia

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DNS and LES of buoyancy-driven turbulence at high Rayleigh numbers: numerical methods and SGS models

F.Xavier Trias[1], X.Álvarez-Farré[1], Daniel Santos[1], Andrey Gorobets[2], Assensi Oliva[1]

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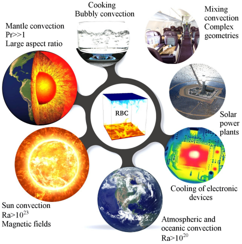
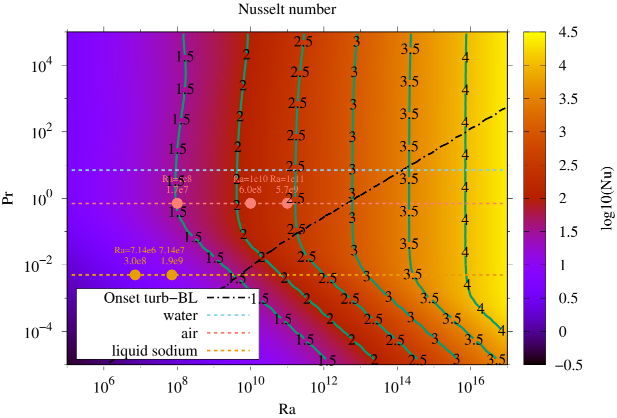
Contents

Motivation

Research question #1:

- Can we hit the ultimate regime of thermal turbulence ?

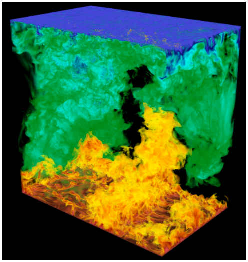


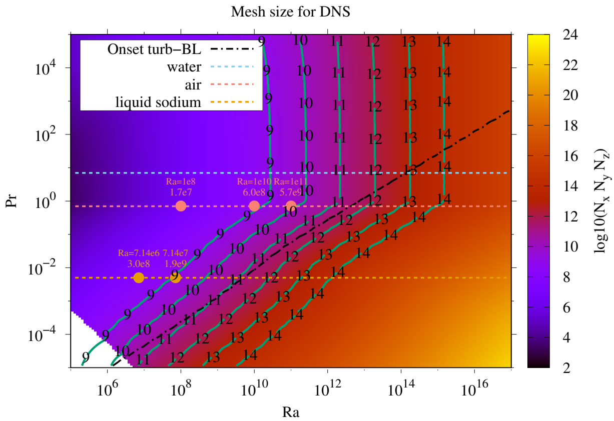


Motivation

Research question #1:

- Can we hit the ultimate regime of thermal turbulence with **DNS**?





Motivation

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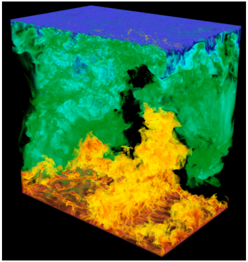
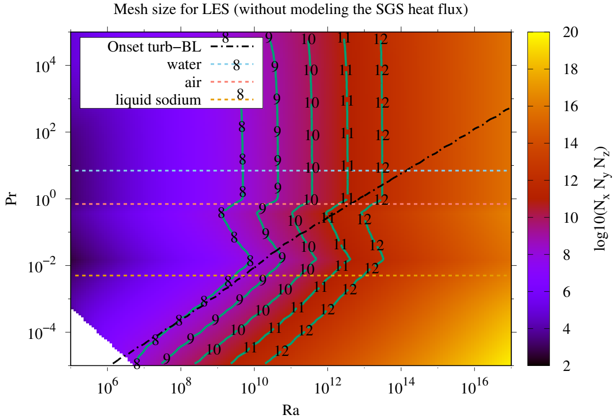
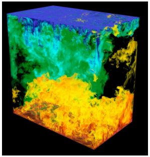


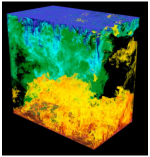


Motivation



DNS $\left\{ \vphantom{\rule{0pt}{10em}} \right.$

Motivation



HAWK | MareNostrum 4 | Marconi100

Rank #27
5,632 nodes with:
2 AMD EPYC 7742
(64 cores each)

Rank #82
3456 nodes with:
2x Intel Xeon 8160
1x Intel Omni-Path

Rank #21
980 nodes with:
2 IBM Power9
4 NVIDIA Volta V100

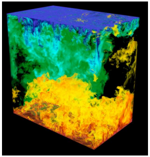
PRACE

intel XEON PLATINUM inside

DNS

HPC (High Performance Computing)

Motivation



How to properly discretize NS?

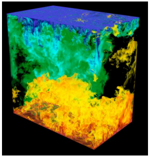
DNS

Numerical Methods

HPC (High Performance Computing)

Motivation

How to properly model SGS?



SGS models

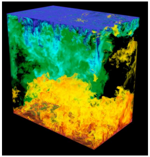
Numerical Methods

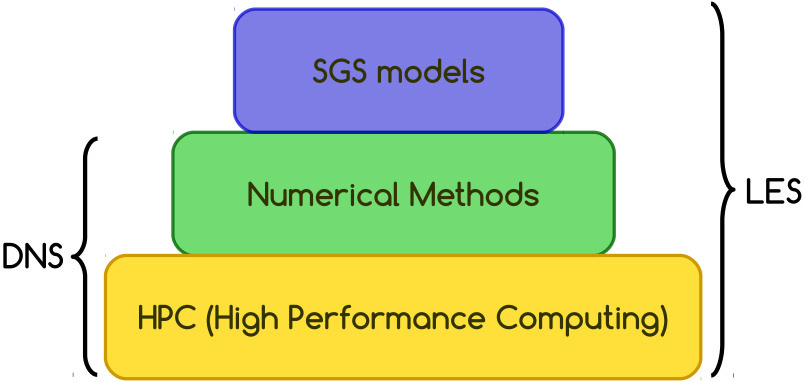
HPC (High Performance Computing)

DNS

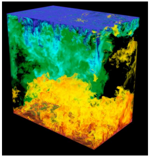
LES

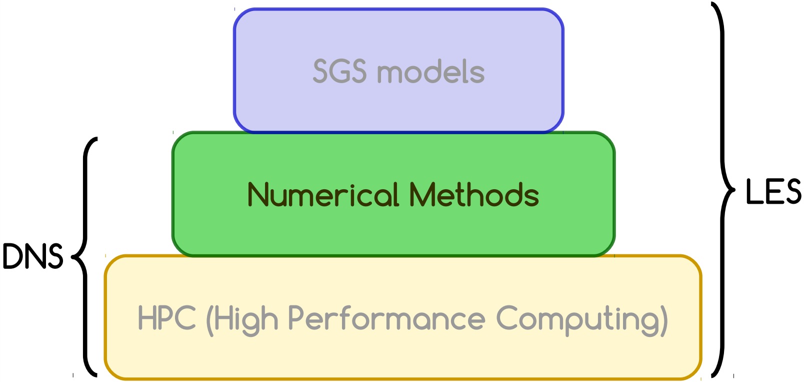
Motivation




SGS models
Numerical Methods
HPC (High Performance Computing)
DNS
LES

Numerical methods for DNS/LES

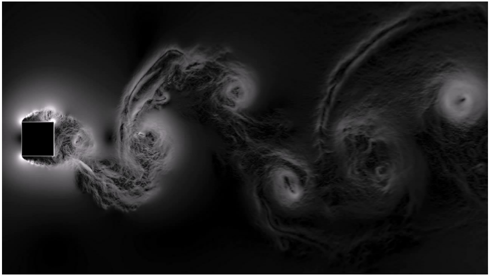


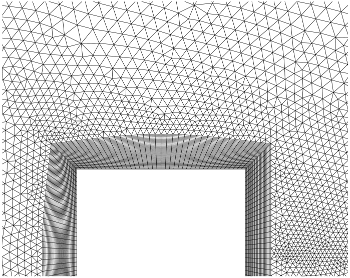


Numerical methods for DNS/LES

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

[1] 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 on unstructured grids[3]

Continuous

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

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

[3] F.X.Trias, O.Lehmkuhl, A.Oliva, C.D.Pérez-Segarra, R.W.C.P.Verstappen. *Symmetry-preserving discretization of Navier-Stokes equations on collocated unstructured grids*, **Journal of Computational Physics**, 258 (1): 246-267, 2014.

Symmetry-preserving discretization on unstructured grids[3]

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

Discrete

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[3] F.X.Trias, O.Lehmkuhl, A.Oliva, C.D.Pérez-Segarra, R.W.C.P.Verstappen. *Symmetry-preserving discretization of Navier-Stokes equations on collocated unstructured grids*, **Journal of Computational Physics**, 258 (1): 246-267, 2014.

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$\langle \nabla \cdot \boldsymbol{a}, \varphi \rangle = -\langle \boldsymbol{a}, \nabla \varphi \rangle$	$\Omega \mathsf{G} = -\mathsf{M}^T$

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$\langle \nabla \cdot \boldsymbol{a}, \varphi \rangle = - \langle \boldsymbol{a}, \nabla \varphi \rangle$	$\Omega \mathsf{G} = -\mathsf{M}^T$
$\left\langle \nabla^2 \boldsymbol{a}, \boldsymbol{b} \right\rangle = \left\langle \boldsymbol{a}, \nabla^2 \boldsymbol{b} \right\rangle$	$\mathsf{D} = \mathsf{D}^T \quad def -$

[3] F.X.Trias, O.Lehmkuhl, A.Oliva, C.D.Pérez-Segarra, R.W.C.P.Verstappen. *Symmetry-preserving discretization of Navier-Stokes equations on collocated unstructured grids*, **Journal of Computational Physics**, 258 (1): 246-267, 2014.

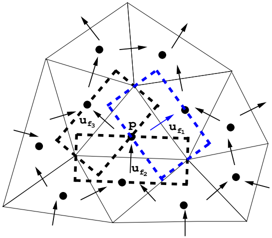
Why collocated arrangements are so popular?

- STAR-CCM+
- ANSYS-FLUENT
- Code-Saturne
- OpenFOAM

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

In staggered meshes

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



4

5

Why collocated arrangements are so popular?

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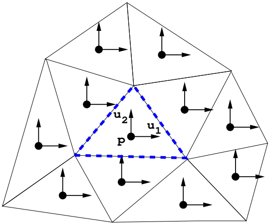
$$\boxed{\Omega_c \frac{d\boldsymbol{u}_c}{dt} + \mathsf{C}\left(\boldsymbol{u}_s\right)\boldsymbol{u}_c = \mathsf{D}\boldsymbol{u}_c - \mathsf{G}_c\boldsymbol{p}_c; \quad \mathsf{M}_c\boldsymbol{u}_c = \boldsymbol{0}_c}$$

In <u>collocated meshes</u>

- p-$\boldsymbol{u}_c$ coupling is cumbersome ✗
- $\mathsf{C}\left(\boldsymbol{u}_s\right)$ and D easy to discretize ✓
- Cheaper, less memory,... ✓



4

5

Why collocated arrangements are so popular?

Everything is easy except the pressure-velocity coupling[4,5]

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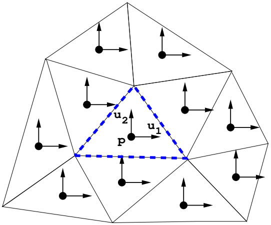
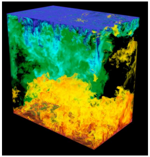
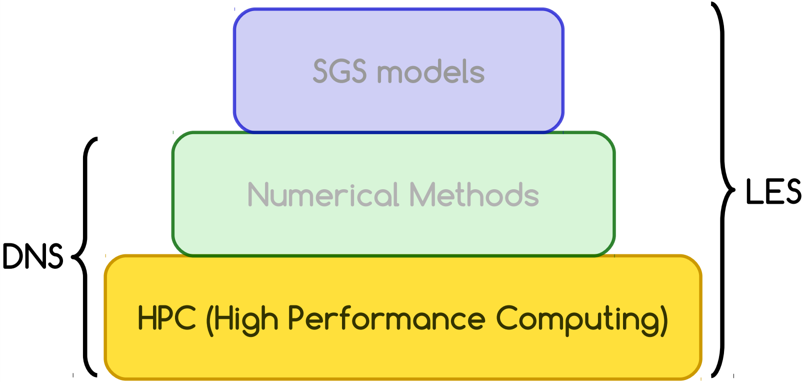


[4] J.A.Hopman, F.X.Trias, J.Rigola. *On a conservative solution to checkerboarding: examining the discrete Laplacian kernel using mesh connectivity* **On Friday at 10:05 in Sala Paolino d'Aquileia**

[5] D.Santos, F.X.Trias, G.Colomer, A.Oliva. *An energy-preserving unconditionally stable fractional step method for DNS/LES on collocated unstructured grids* **On Friday at 10:20 in Sala Paolino d'Aquileia**

HPC on modern supercomputers

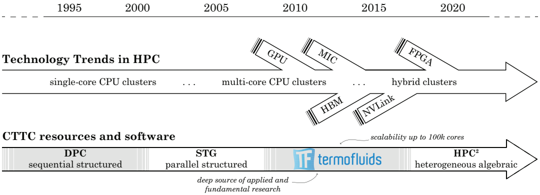




HPC on modern supercomputers

Research question #3:

- How can we develop **portable** and **efficient** CFD codes for large-scale simulations on modern supercomputers?



[6] X.Álvarez, A.Gorobets, F.X.Trias. *A hierarchical parallel implementation for heterogeneous computing. Application to algebra-based CFD simulations on hybrid supercomputers*. **Computers & Fluids**, 214:104768, 2021

[7] À.Alsalti, X.Álvarez, F.X.Trias, A.Oliva. *Exploiting spatial symmetries for solving Poisson's equation* (submitted).

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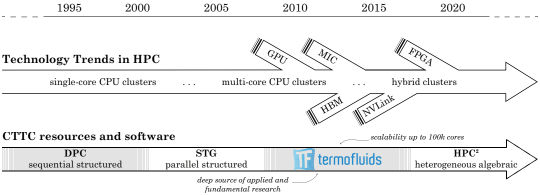

HPC^2: portable, algebra-based framework for heterogeneous computing is being developed[6]. Traditional stencil-based data and sweeps are replaced by algebraic structures (sparse matrices and vectors) and kernels. `SpMM`-based strategies to increase the arithmetic intensity are under development[7].

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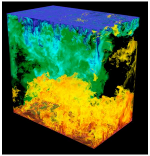
LES of RBC



SGS models

Numerical Methods

HPC (High Performance Computing)

DNS

LES

Problems to model the SGS heat flux[8]

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

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

$$\boxed{\nu_t \approx (C_m \delta)^2 D_m(\overline{\boldsymbol{u}})} \quad \longrightarrow \quad \{\text{WALE, Vreman, QR, Sigma, S3PQR,...}\}$$

[8]F.Dabbagh, F.X.Trias, A.Gorobets, A.Oliva. *A priori study of subgrid-scale features in turbulent Rayleigh-Bénard convection*, **Physics of Fluids**, 29:105103, 2017.

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$$\partial_t \overline{T} + (\overline{\boldsymbol{u}} \cdot \nabla)\overline{T} = \alpha \nabla^2 \overline{T} - \nabla \cdot \boldsymbol{q} \quad \text{where} \quad \boldsymbol{q} = \overline{\boldsymbol{u}T} - \overline{\boldsymbol{u}}\,\overline{T}$$

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eddy-diffusivity

$$\boldsymbol{q} \approx -\alpha_t \nabla \overline{T} \qquad (\equiv \boldsymbol{q}^{eddy})$$

gradient model

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

[8] F.Dabbagh, F.X.Trias, A.Gorobets, A.Oliva. *A priori study of subgrid-scale features in turbulent Rayleigh-Bénard convection*, **Physics of Fluids**, 29:105103, 2017.

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eddy-diffusivity

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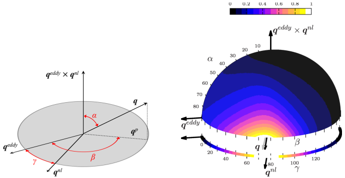

[8] F.Dabbagh, F.X.Trias, A.Gorobets, A.Oliva. *A priori study of subgrid-scale features in turbulent Rayleigh-Bénard convection*, **Physics of Fluids**, 29:105103, 2017.

Problems to model the SGS heat flux[8]

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

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

$\boxed{\nu_t \approx (C_m \delta)^2 D_m(\overline{\boldsymbol{u}})}$ $\longrightarrow$ {WALE, Vreman, QR, Sigma, S3PQR,... }

$$\partial_t \overline{T} + (\overline{\boldsymbol{u}} \cdot \nabla)\overline{T} = \alpha \nabla^2 \overline{T} - \nabla \cdot \boldsymbol{q} \quad \text{where} \quad \boldsymbol{q} = \overline{\boldsymbol{u}T} - \overline{\boldsymbol{u}}\,\overline{T}$$

eddy-diffusivity

$$\cancel{\boldsymbol{q} \approx -\alpha_t \nabla \overline{T}} \qquad (\equiv \boldsymbol{q}^{eddy})$$

gradient model

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

[8] F.Dabbagh, F.X.Trias, A.Gorobets, A.Oliva. *A priori study of subgrid-scale features in turbulent Rayleigh-Bénard convection*, **Physics of Fluids**, 29:105103, 2017.

DNS results at very low Pr number

Why? scale separation grows as $\eta_K/\eta_T = Pr^{3/4}$.

η_T: Obukhov-Corrsin scale; η_K: Kolmogorov scale

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Why? scale separation grows as $\eta_K/\eta_T = Pr^{3/4}$. $\boxed{\text{Here: } \eta_T \approx 53.2\eta_K}$

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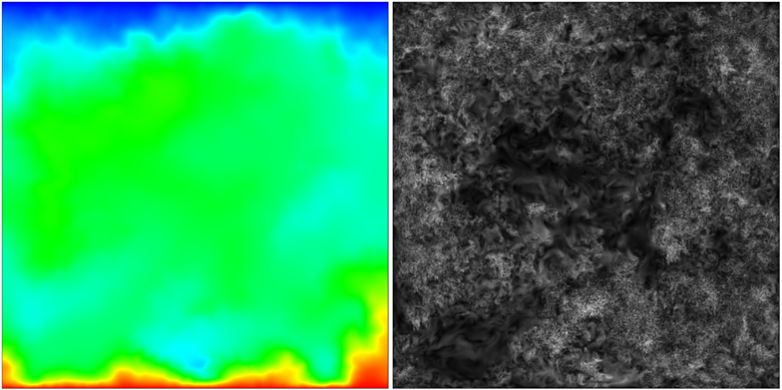

DNS of a RB at $Ra = 7.14 \times 10^6$ and $Pr = 0.005$ (liquid sodium)

$488 \times 488 \times 1280 \approx$ **305M**

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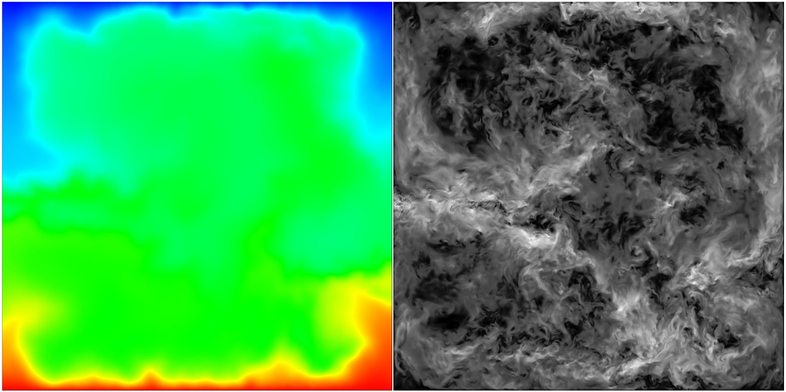

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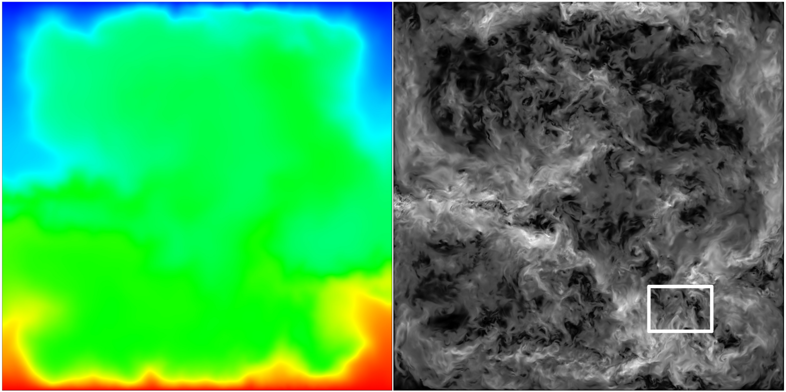

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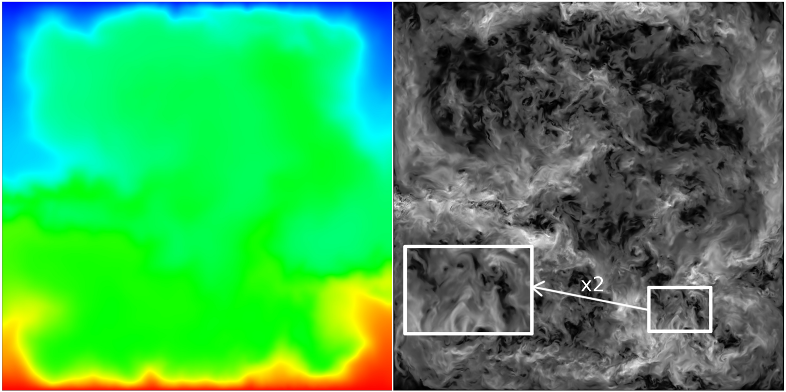

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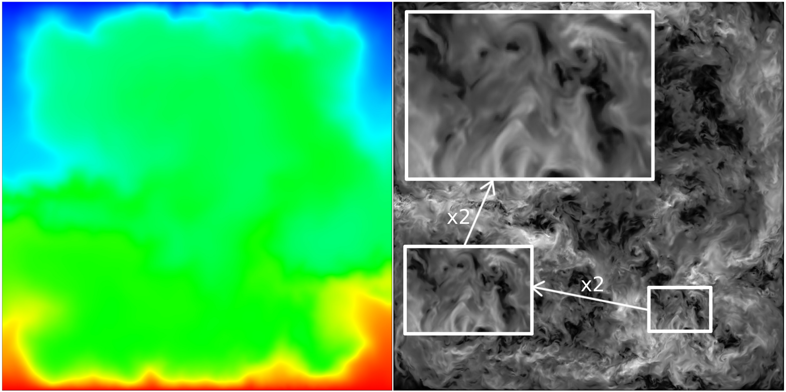

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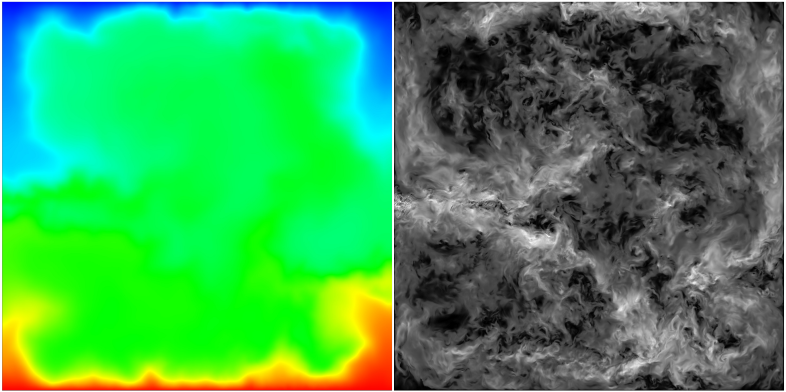

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DNS vs LES results at very low Pr number[9]

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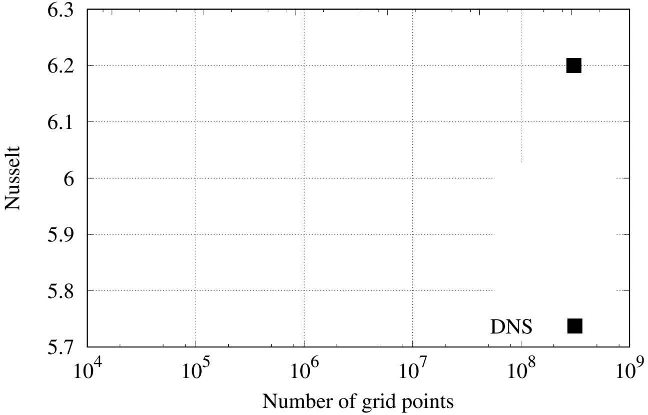

[9] F.X.Trias, F.Dabbagh, A.Gorobets, C.Oliet. *On a proper tensor-diffusivity model for LES of buoyancy-driven turbulence*, **Flow Turbul Combust**, 105:393-414, 2020.

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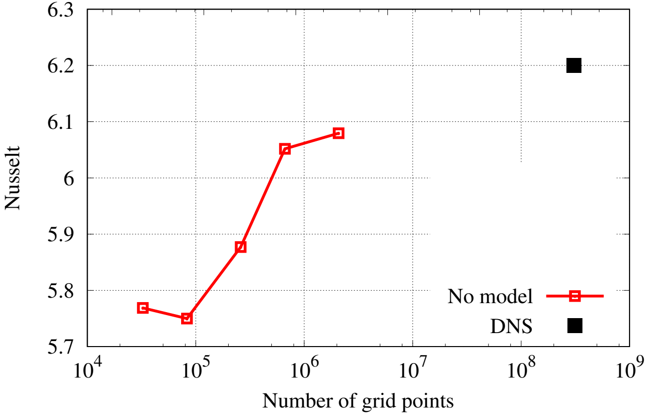

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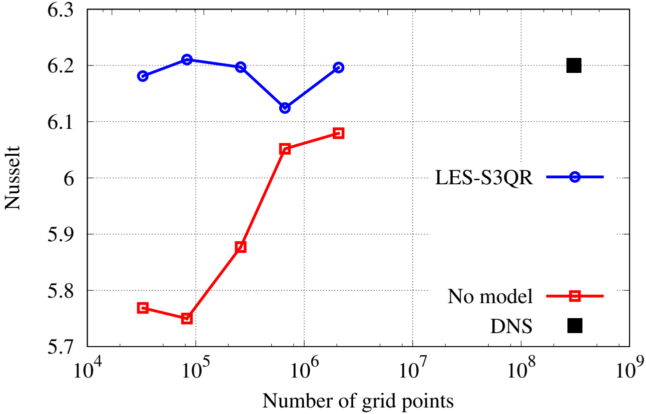

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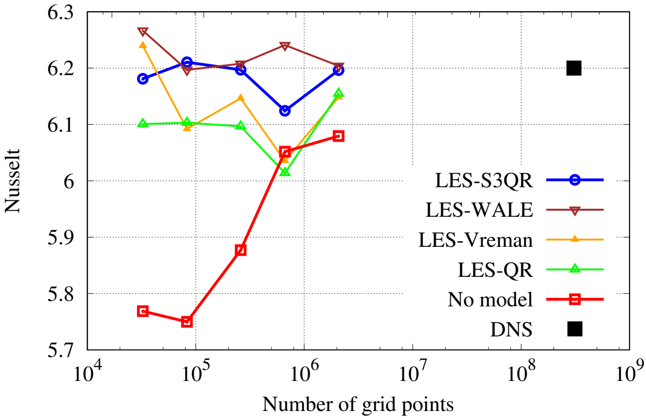

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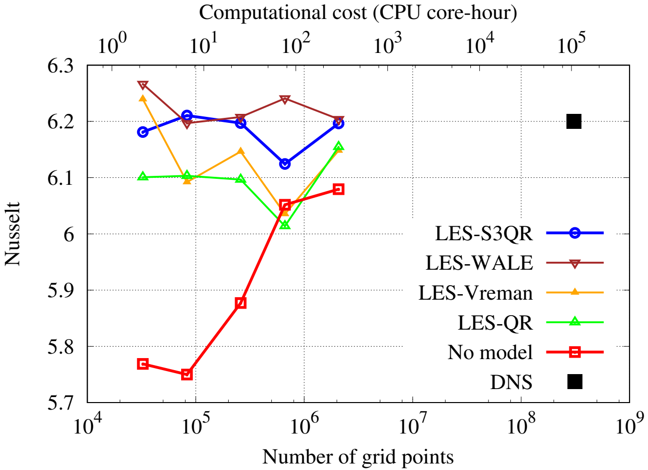

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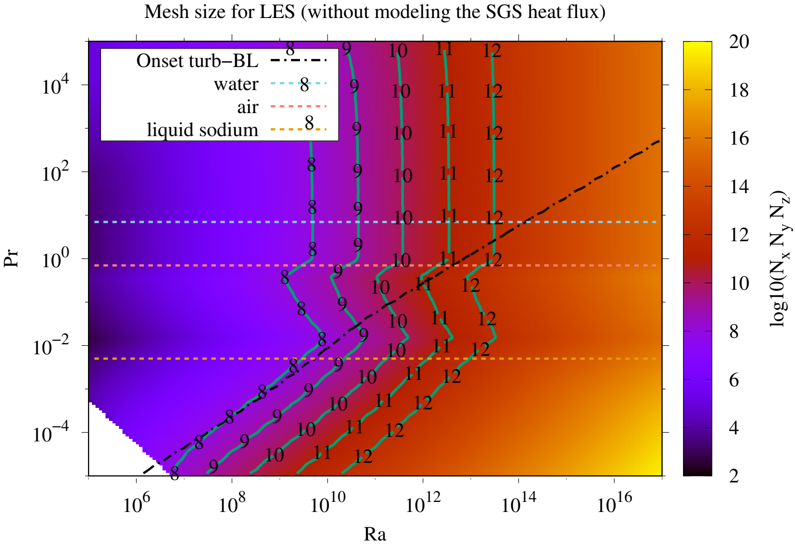
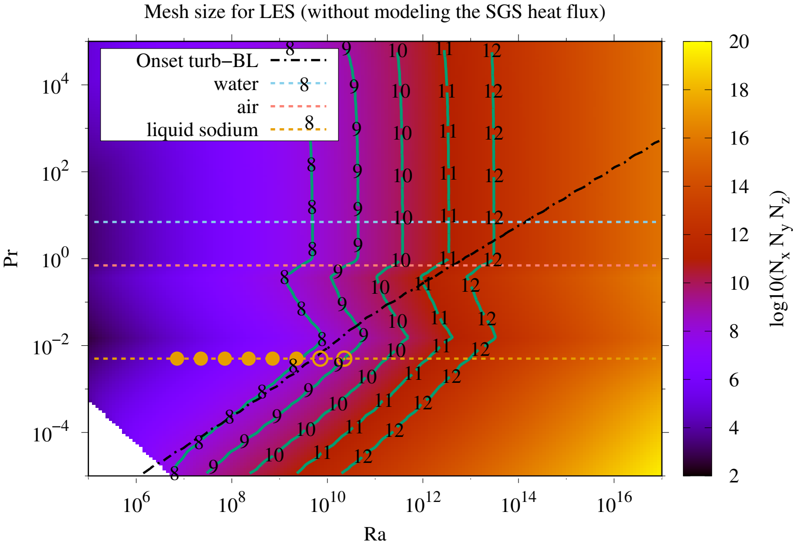
LES results at very low *Pr* number



LES results at very low *Pr* number (on-going)



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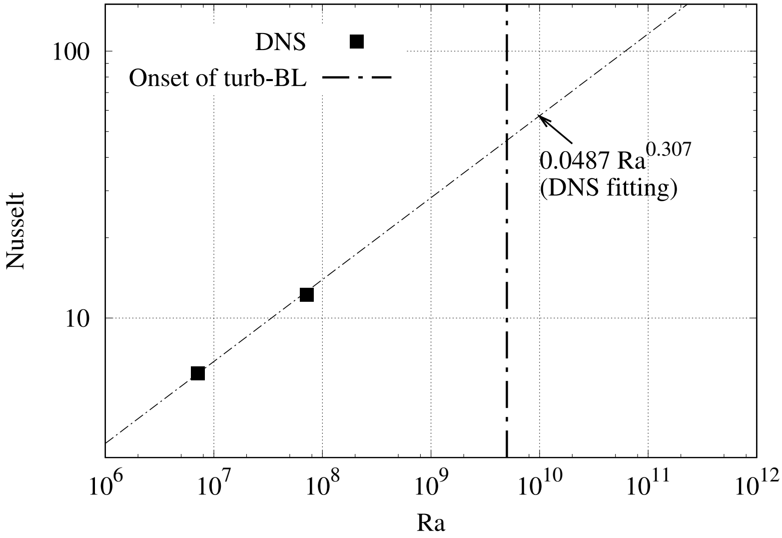

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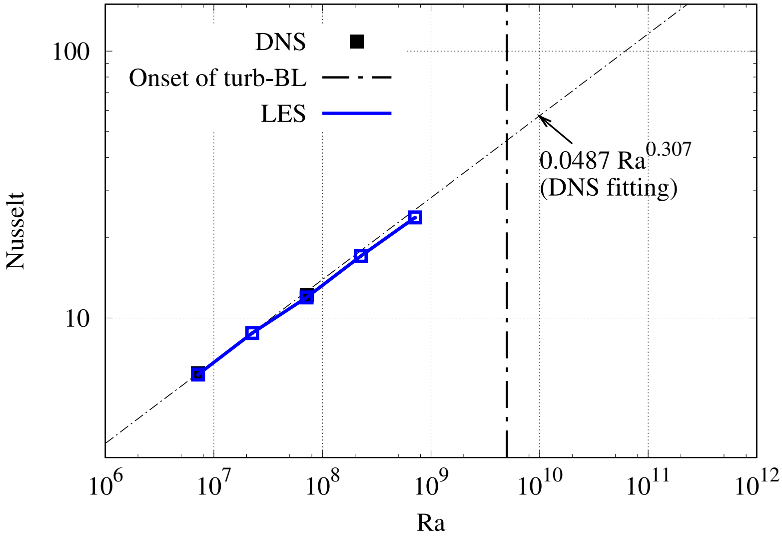

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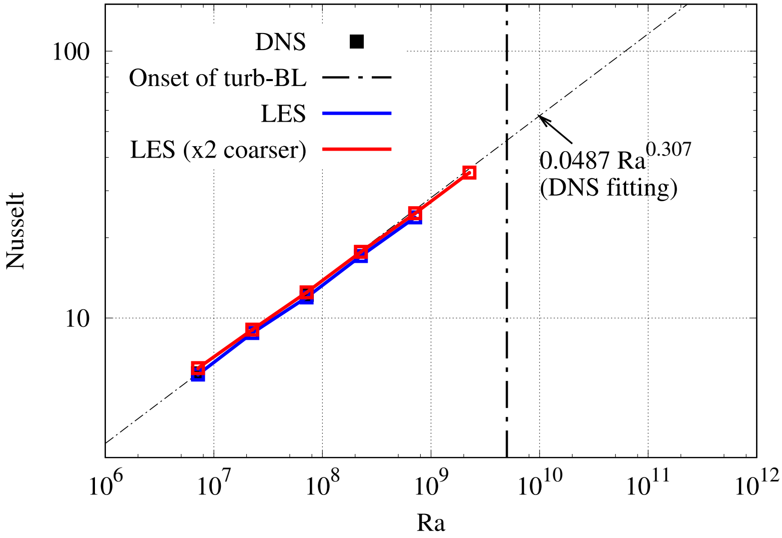
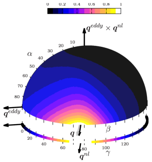


Concluding remarks

- Modeling the SGS heat flux, $\boldsymbol{q}$, is the main difficulty for LES of buoyancy-driven flows



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- Modeling the SGS heat flux, $\boldsymbol{q}$, is the main difficulty for LES of buoyancy-driven flows
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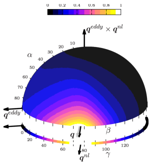

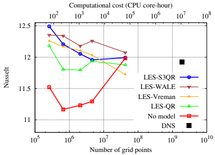

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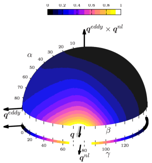

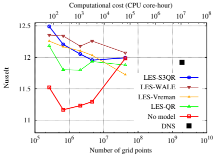

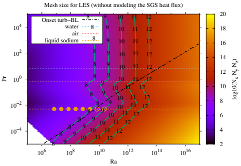

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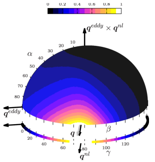
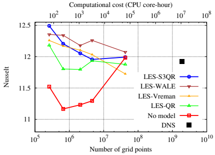
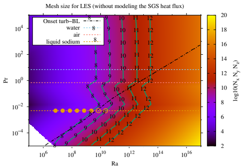




On-going research:

- LES simulations at low-*Pr* and very large *Ra*
- Re-thinking standard CFD operators (*e.g* flux limiters[a], boundary conditions, CFL,...) to adapt them into an algebraic framework



[a] N.Valle, X.Álvarez, A.Gorobets, J.Castro, A.Oliva, F.X.Trias. *On the implementation of flux limiters in algebraic frameworks*. **Computer Physics Communications**, 271:108230, 2022.

Thank you for your ~~virtual~~ attendance