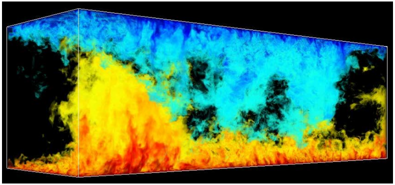
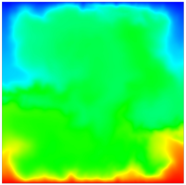
Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

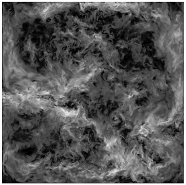
Can we hit the ultimate regime of thermal turbulence using LES simulations at low Prandtl numbers?

F.Xavier Trias[1], Andrey Gorobets[2], Assensi Oliva[1]
Presenter: Jesús Ruano[1]

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





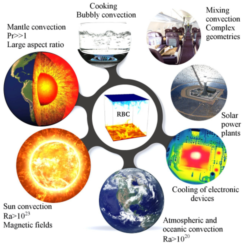


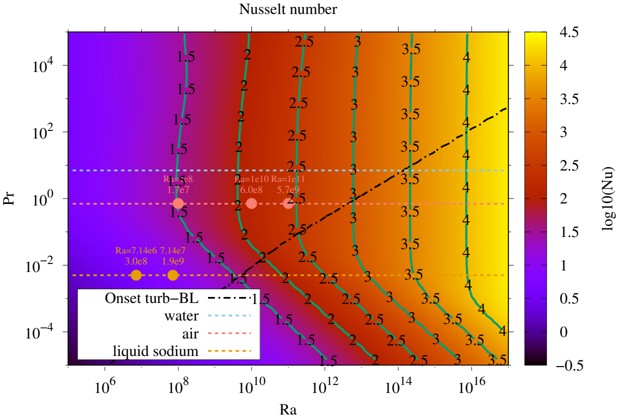
Contents

Motivation

Research question #1:

- Can we hit the ultimate regime of thermal turbulence ?

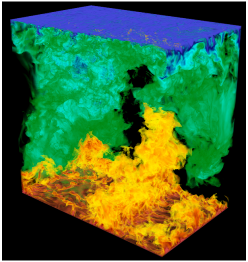


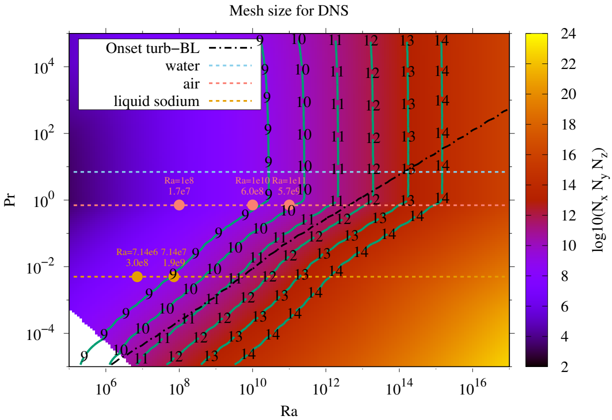


Motivation

Research question #1:

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

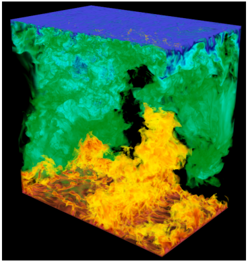


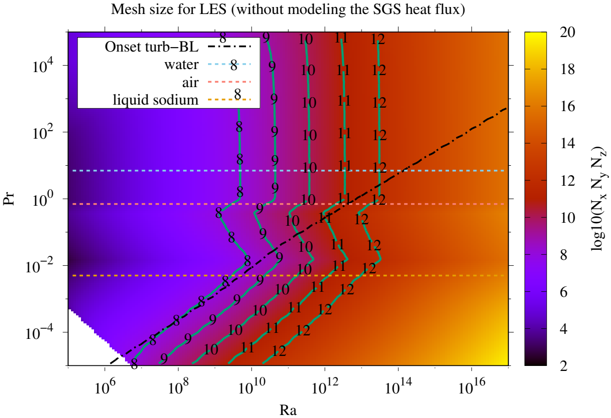


Motivation

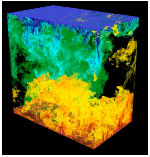
Research question #1:

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



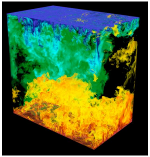


Motivation



DNS

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

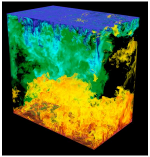
PRACE

intel XEON PLATINUM inside

DNS

HPC (High Performance Computing)

Motivation

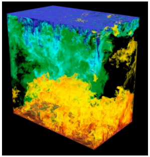


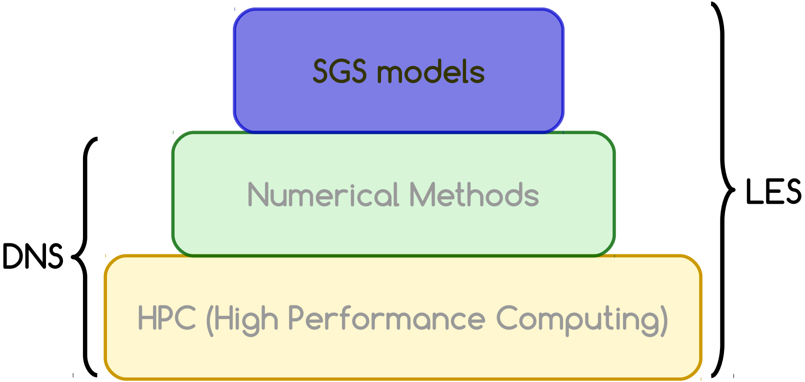
How to properly discretize NS?

DNS {
- Numerical Methods
- HPC (High Performance Computing)

Motivation

How to properly model SGS?





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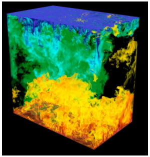
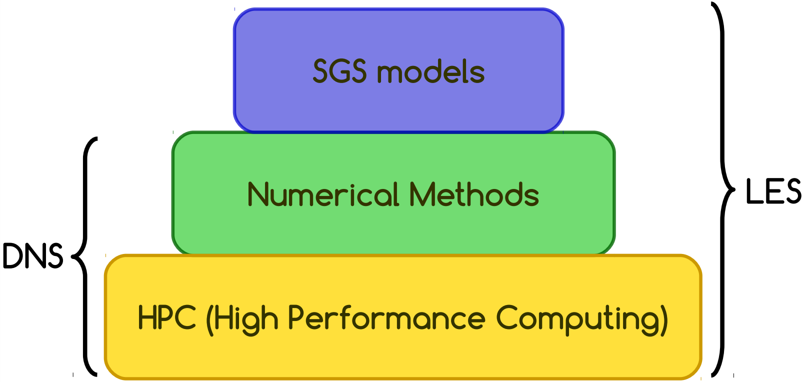
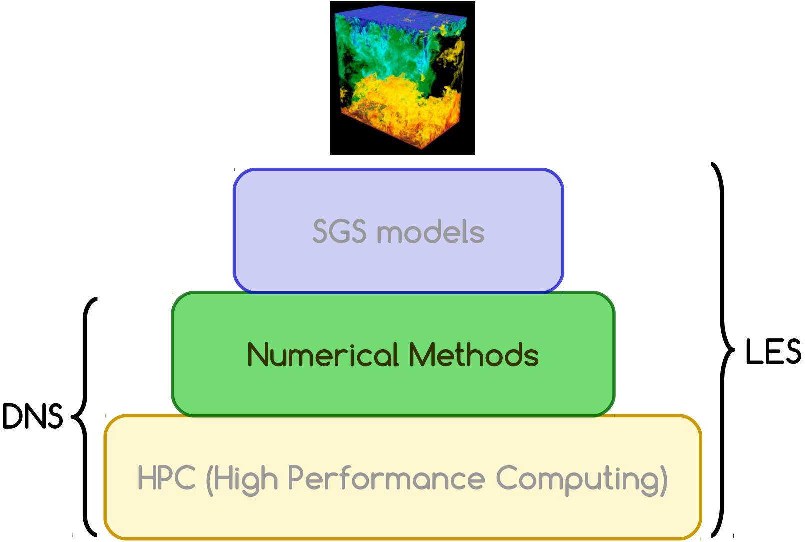



SGS models
Numerical Methods
HPC (High Performance Computing)
DNS
LES

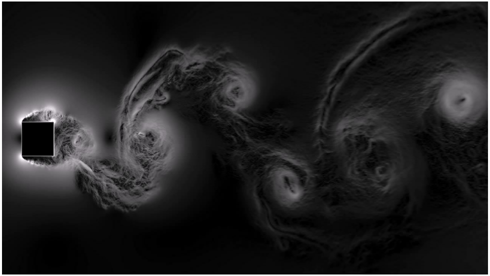
Numerical methods for DNS/LES

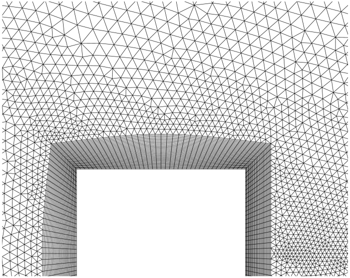


Numerical methods for DNS/LES

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.

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Discrete

$$\Omega \frac{d\boldsymbol{u}_h}{dt} + \mathsf{C}(\boldsymbol{u}_h)\,\boldsymbol{u}_h = \mathsf{D}\boldsymbol{u}_h - \mathsf{G}\boldsymbol{p}_h$$

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$$\langle \boldsymbol{a}, \boldsymbol{b} \rangle = \int_\Omega \boldsymbol{a}\boldsymbol{b} d\Omega$$

Discrete

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$$\langle \boldsymbol{a}_h, \boldsymbol{b}_h \rangle_h = \boldsymbol{a}_h^T \Omega \boldsymbol{b}_h$$

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$\langle \boldsymbol{a}, \boldsymbol{b} \rangle = \int_\Omega \boldsymbol{a}\boldsymbol{b} d\Omega$	$\langle \boldsymbol{a}_h, \boldsymbol{b}_h \rangle_h = \boldsymbol{a}_h^T \Omega \boldsymbol{b}_h$
$\langle C(\boldsymbol{u}, \varphi_1), \varphi_2 \rangle = -\langle C(\boldsymbol{u}, \varphi_2), \varphi_1 \rangle$	$\mathsf{C}(\boldsymbol{u}_h) = -\mathsf{C}^T(\boldsymbol{u}_h)$

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

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

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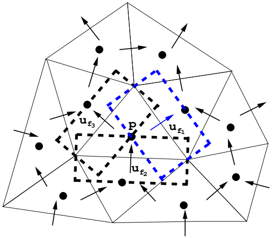
Why collocated arrangements are so popular?

- STAR-CCM+ — CD-adapco, SIEMENS
- ANSYS-FLUENT — ANSYS FLUENT®
- Code-Saturne — CODE SATURNE, eDF, GPL
- OpenFOAM — Open∇FOAM®, GPL 3 Free Software

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

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

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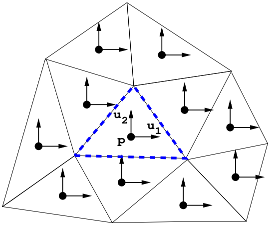
$$\Omega_c \frac{d\boldsymbol{u}_c}{dt} + \mathsf{C}\left(\boldsymbol{u}_s\right)\boldsymbol{u}_c = \mathsf{D}\boldsymbol{u}_c - \mathsf{G}_c\boldsymbol{p}_c; \quad \mathsf{M}_c\boldsymbol{u}_c = \mathbf{0}_c$$

In collocated meshes

- 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]

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

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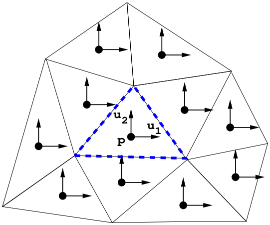
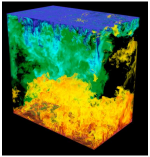
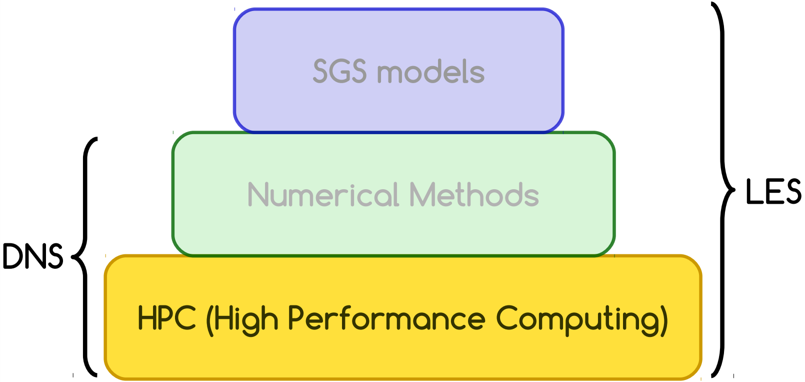


[4] J.A.Hopman, À.Alsalti, F.X.Trias, J.Rigola. *On a checkerboard-free, conservative method for turbulent flows* **On Thursday at 16h in Cloister**

[5] D.Santos, F.X.Trias, J.A.Hopman, C.D.Pérez-Segarra. *Pressure-velocity coupling on unstructured collocated grids: reconciling stability and energy-conservation* **On Wednesday at 14:50 in Room B**

HPC on modern supercomputers

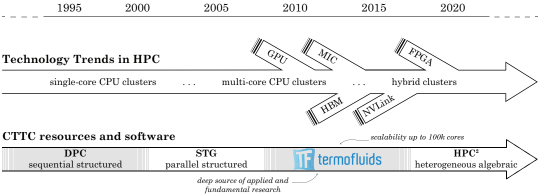




HPC on modern supercomputers

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* **Journal of Computational Physics**, 486:112133, 2023.

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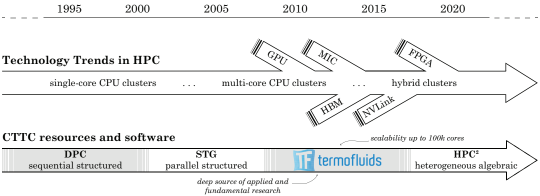

HPC^2: portable, algebra-based framework for heterogeneous computing is being developed[6]. Traditional stencil-based data and sweeps are replaced by algebraic structures (sparse matrices and vectors) and kernels. `SpMM`-based strategies to increase the arithmetic intensity are under development[7].

[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

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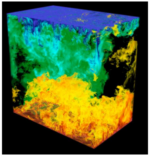
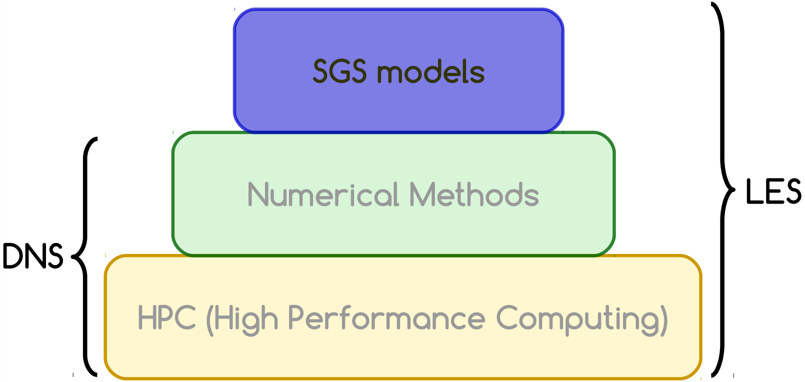
LES of RBC




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

Problems to model the SGS heat flux[8]

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

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

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

[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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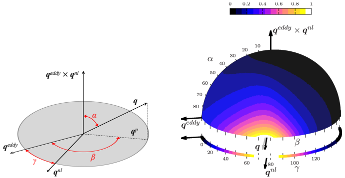
eddy-diffusivity

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



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

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

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

eddy-diffusivity

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

gradient model

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

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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 $\eta_K/\eta_T = Pr^{3/4}$. Here: $\eta_T \approx 53.2\eta_K$

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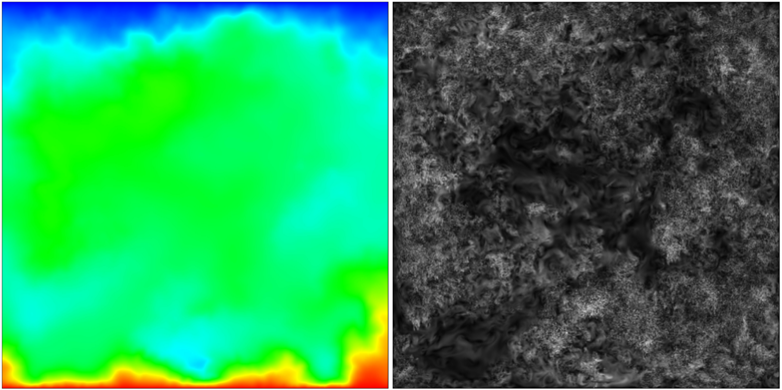

DNS of a RB at $Ra = 7.14 \times 10^6$ and $Pr = 0.005$ (liquid sodium)

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

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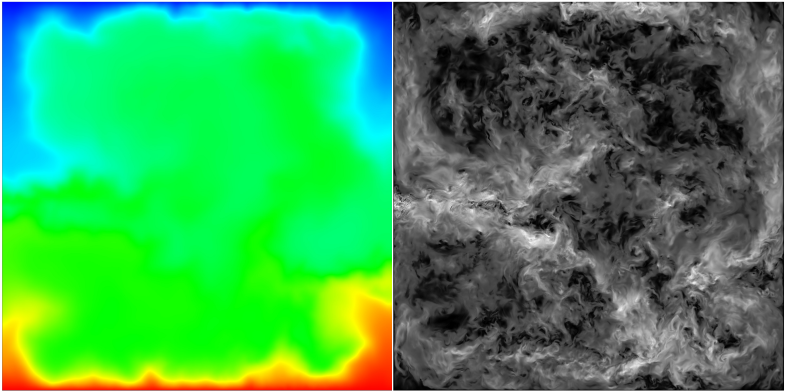

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$966 \times 966 \times 2048 \approx$ **1911M**

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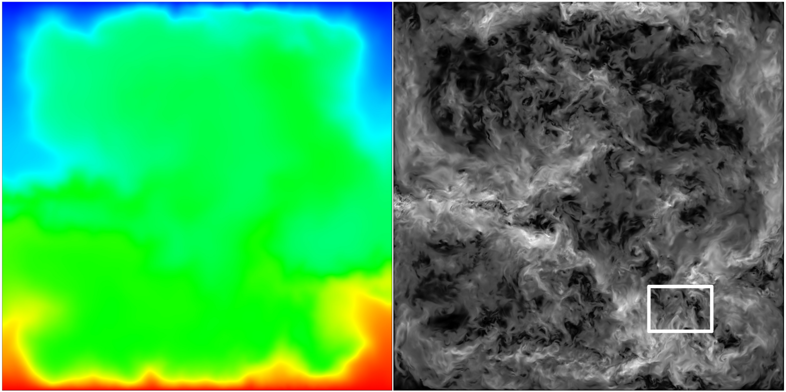

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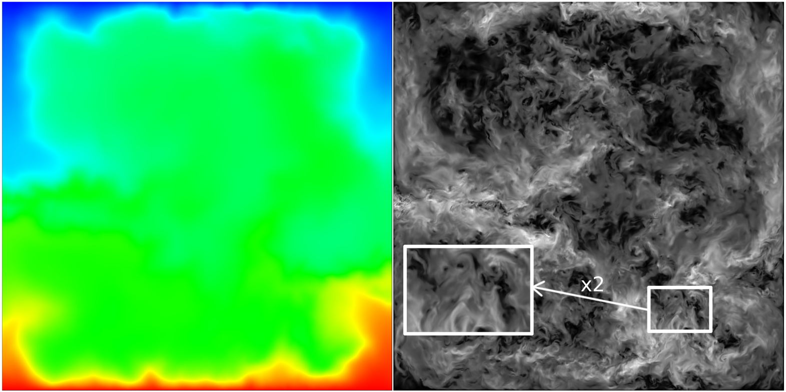

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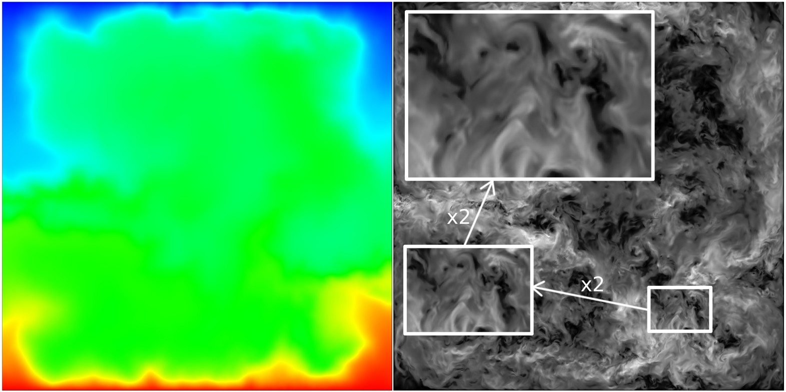

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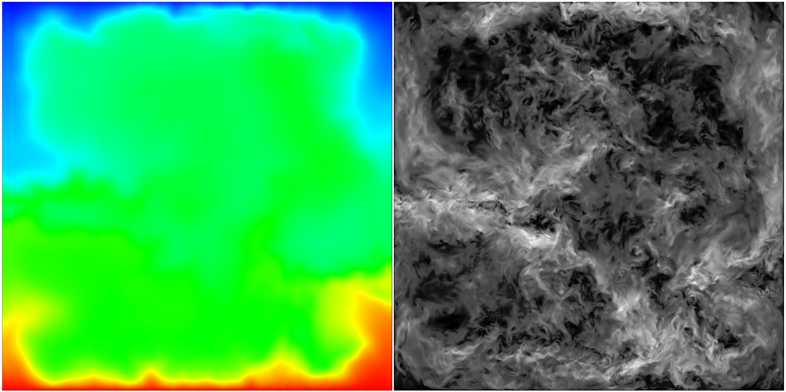

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DNS vs LES results at very low Pr number[9]

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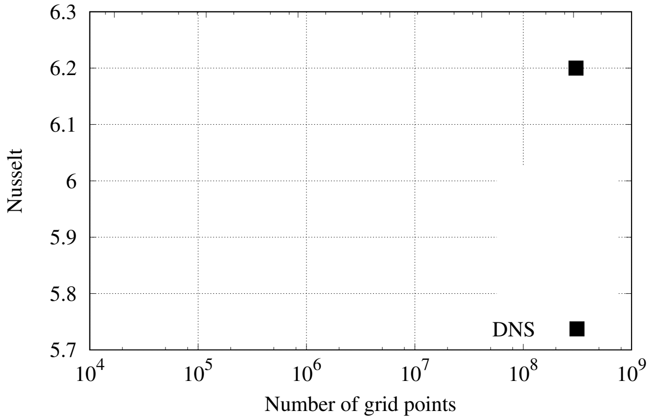

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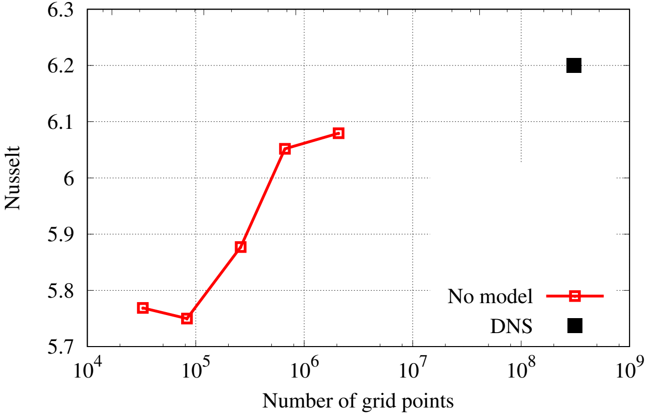

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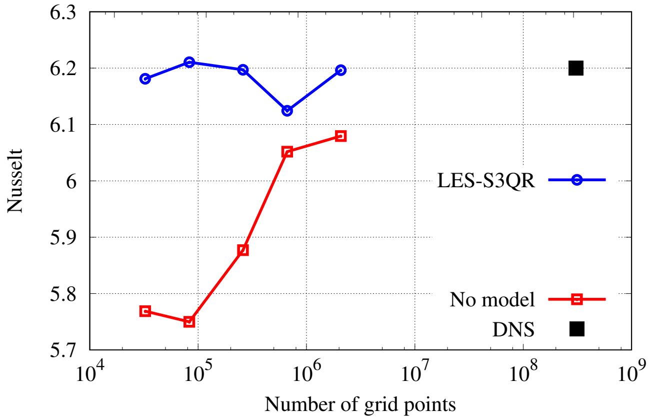

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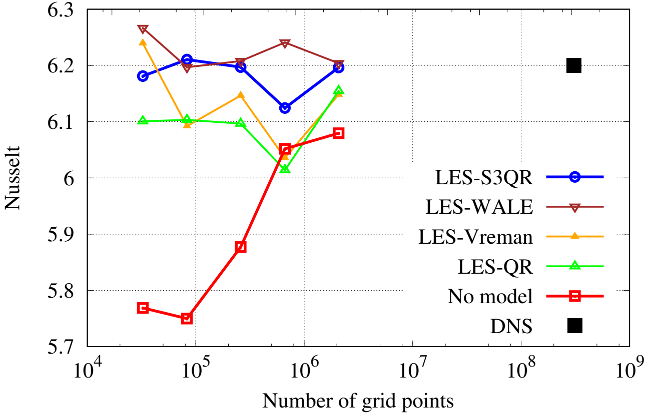

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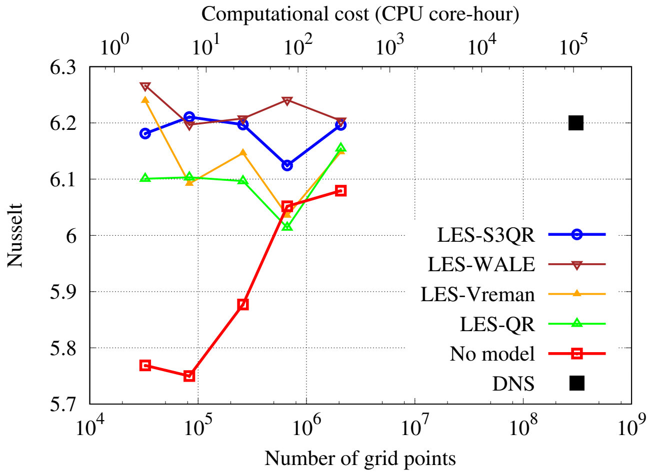

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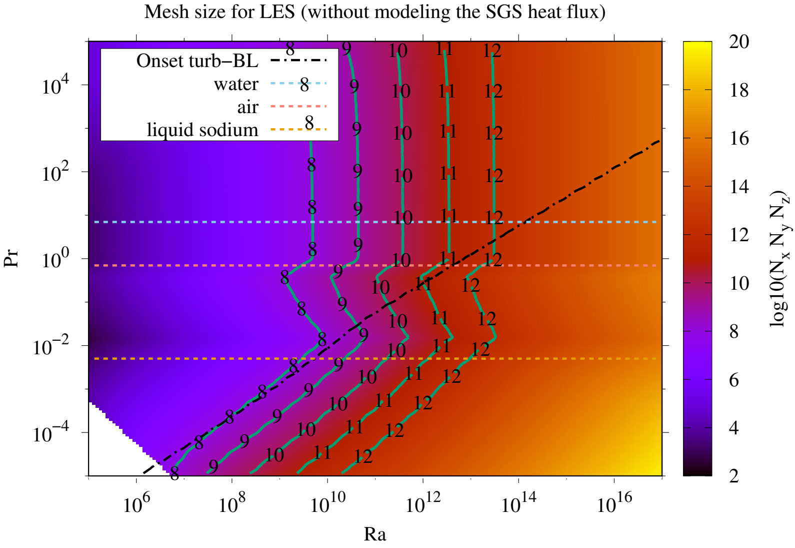
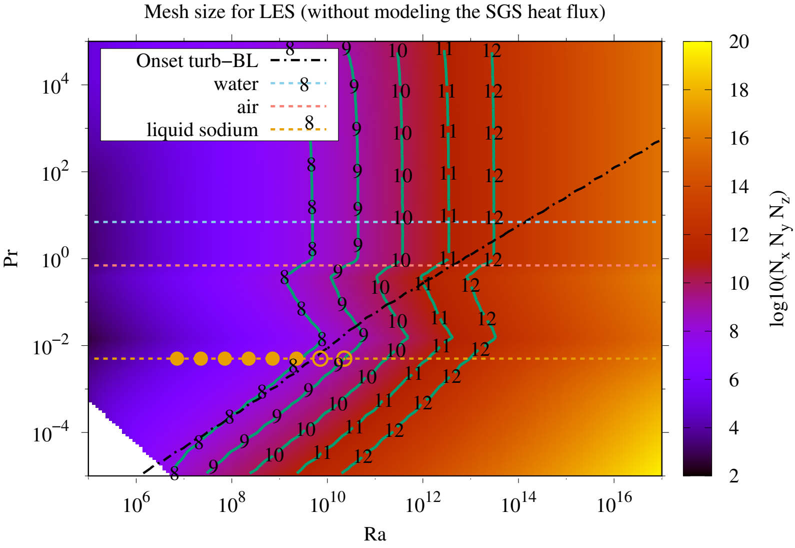
LES results at very low *Pr* number



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



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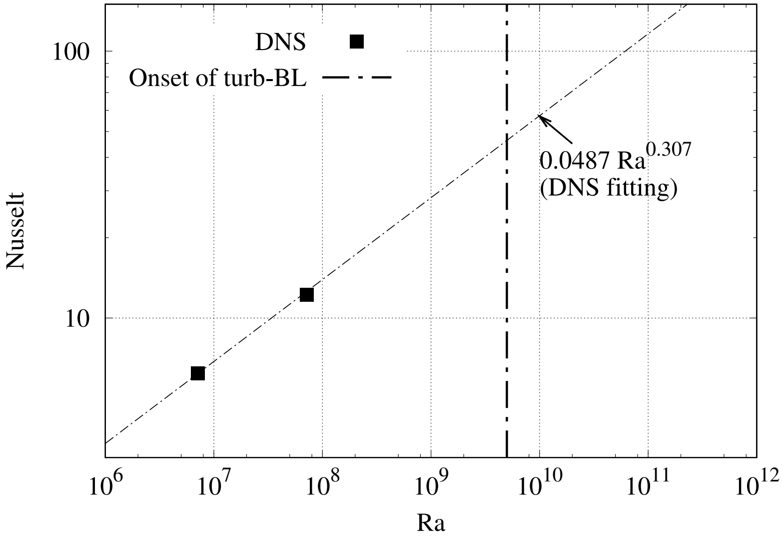

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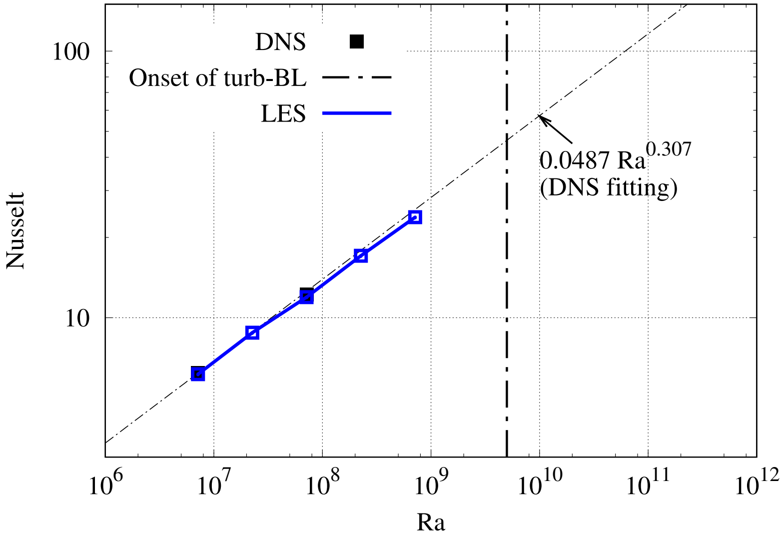

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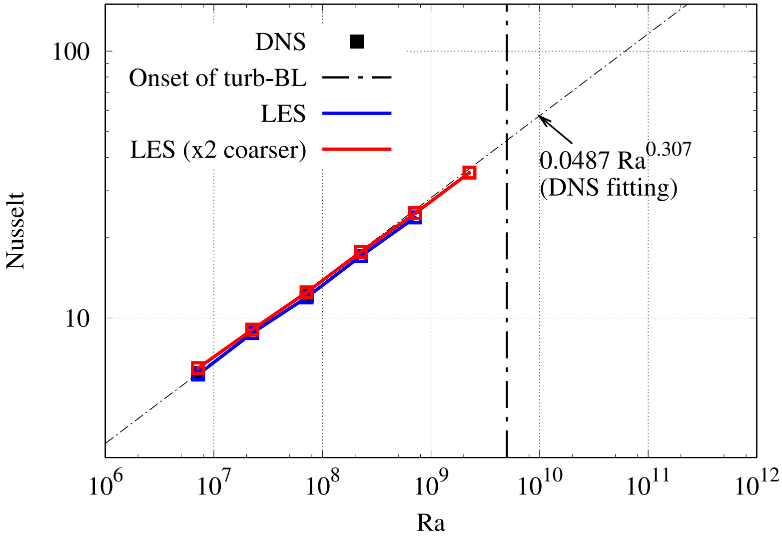
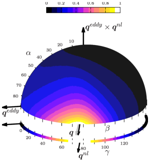


Concluding remarks

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



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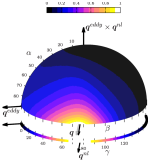

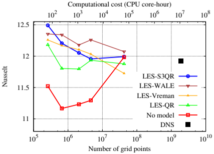

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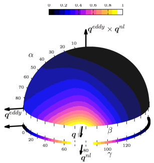

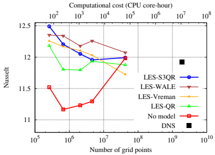

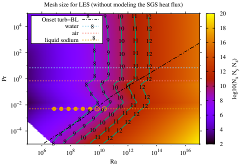

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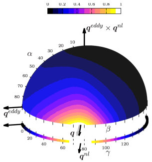
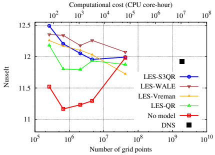
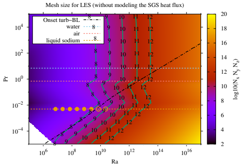




On-going research:

- 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 attendance