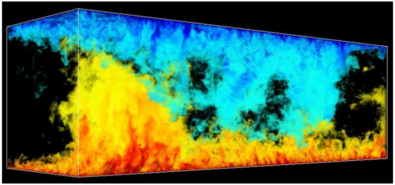
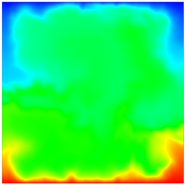
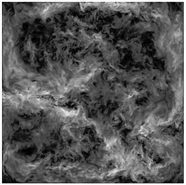
Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

termofluids

Can we hit the ultimate regime of thermal turbulence using large-scale LES simulations?

F. Xavier Trias[1]

[1]Heat and Mass Transfer Technological Center, Technical University of Catalonia
[2]Termo Fluids S.L. Carrer de Magí Colet 8, 08204 Sabadell (Barcelona), Spain

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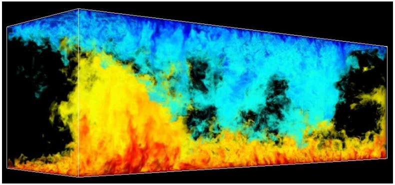
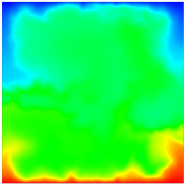
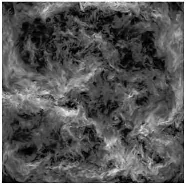

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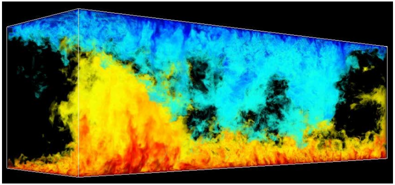
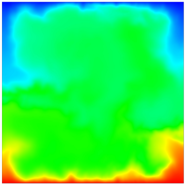
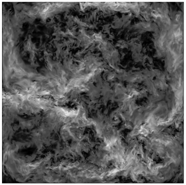
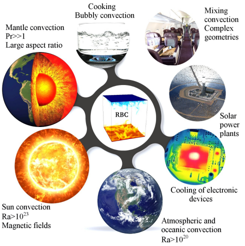




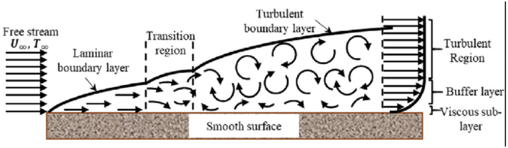
Contents

Motivation

Research question #1:

- Can we hit the ultimate regime of thermal turbulence ?





[1] Robert H. Kraichnan. *Turbulent Thermal Convection at Arbitrary Prandtl Number*, **Physics of Fluids**, 1374–1389, 1962.

Motivation

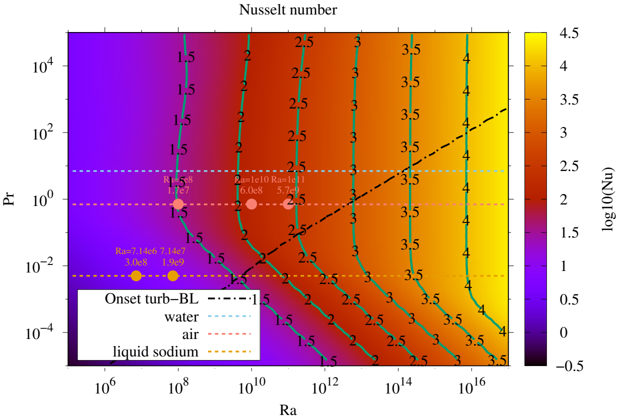
Research question #1:

- Can we hit the ultimate regime of thermal turbulence ?

$$\mathrm{Pr} = \frac{\text{Momentum diffusivity}}{\text{Thermal diffusivity}}$$

$$\mathrm{Ra} = \frac{\text{Buoyancy}}{\text{Diffusivity}}$$

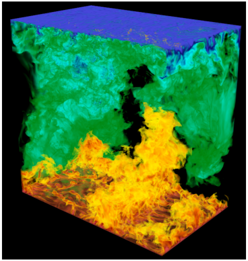
$$\mathrm{Nu} = \frac{\text{Convective heat transfer}}{\text{Conductive heat transfer}}$$

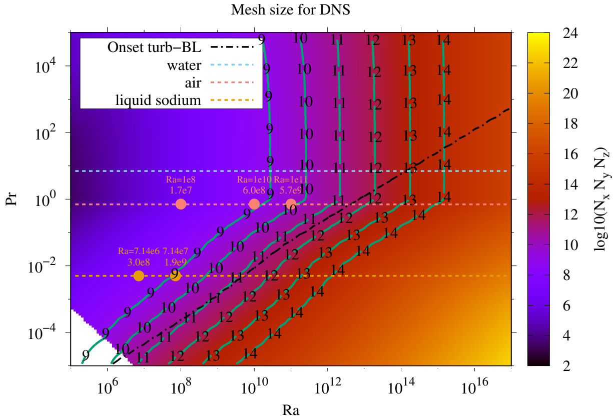


Motivation

Research question #1:

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

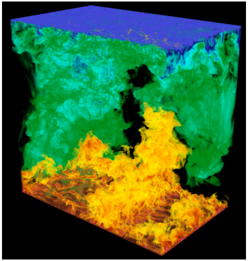


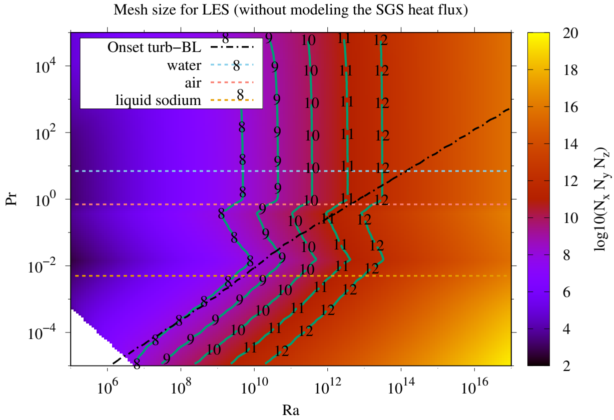


Motivation

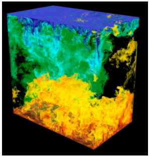
Research question #1:

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



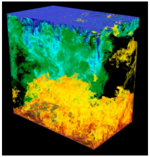


Motivation



DNS

Motivation



HAWK

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

MareNostrum 4

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

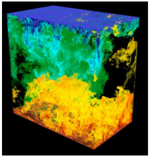
Marconi100

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

DNS

HPC (High Performance Computing)

Motivation



How to properly discretize NS?

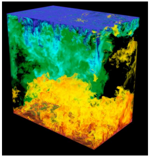
DNS

Numerical Methods

HPC (High Performance Computing)

Motivation

How to properly model SGS?



SGS models

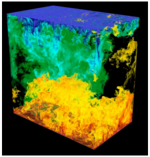
Numerical Methods

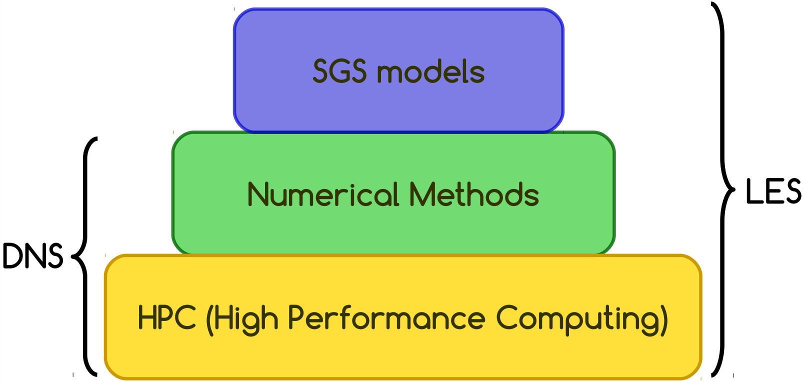
HPC (High Performance Computing)

DNS

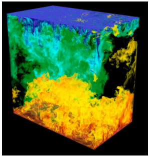
LES

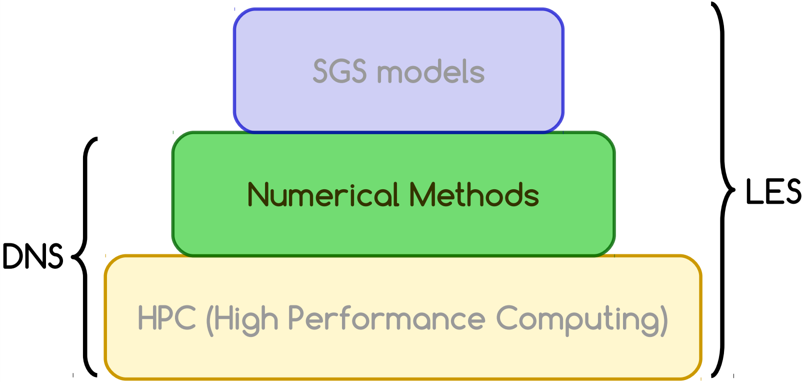
Motivation




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

Numerical methods for DNS/LES

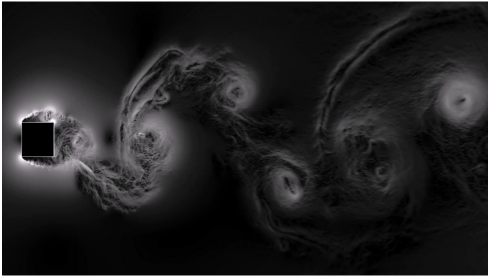


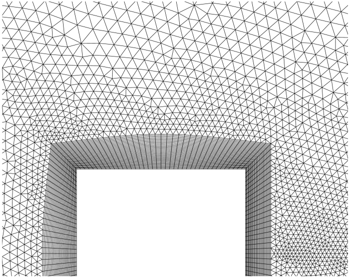


Numerical methods for DNS/LES

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

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

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

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

[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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$\langle \boldsymbol{a}, \boldsymbol{b} \rangle = \int_\Omega \boldsymbol{a}\boldsymbol{b}\, d\Omega$	$\langle \boldsymbol{a}_h, \boldsymbol{b}_h \rangle_h = \boldsymbol{a}_h^T \Omega \boldsymbol{b}_h$

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

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

$$\langle C(\boldsymbol{u}, \varphi_1), \varphi_2 \rangle = - \langle C(\boldsymbol{u}, \varphi_2), \varphi_1 \rangle$$

Discrete

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

$$\mathsf{M}\boldsymbol{u}_h = \boldsymbol{0}_h$$

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

$$\mathsf{C}(\boldsymbol{u}_h) = -\mathsf{C}^T(\boldsymbol{u}_h)$$

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$\langle C(\boldsymbol{u}, \varphi_1), \varphi_2 \rangle = - \langle C(\boldsymbol{u}, \varphi_2), \varphi_1 \rangle$	$\mathsf{C}(\boldsymbol{u}_h) = -\mathsf{C}^T(\boldsymbol{u}_h)$
$\langle \nabla \cdot \boldsymbol{a}, \varphi \rangle = - \langle \boldsymbol{a}, \nabla \varphi \rangle$	$\Omega \mathsf{G} = -\mathsf{M}^T$

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$\langle C(\boldsymbol{u}, \varphi_1), \varphi_2 \rangle = -\langle C(\boldsymbol{u}, \varphi_2), \varphi_1 \rangle$	$\mathsf{C}(\boldsymbol{u}_h) = -\mathsf{C}^T(\boldsymbol{u}_h)$
$\langle \nabla \cdot \boldsymbol{a}, \varphi \rangle = -\langle \boldsymbol{a}, \nabla \varphi \rangle$	$\Omega \mathsf{G} = -\mathsf{M}^T$
$\left\langle \nabla^2 \boldsymbol{a}, \boldsymbol{b} \right\rangle = \left\langle \boldsymbol{a}, \nabla^2 \boldsymbol{b} \right\rangle$	$\mathsf{D} = \mathsf{D}^T \quad def -$

[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.

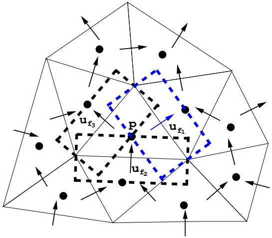
Why collocated arrangements are so popular?

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

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

In staggered meshes

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



Why collocated arrangements are so popular?

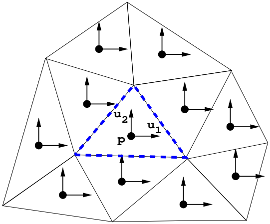
Everything is easy except the pressure-velocity coupling

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

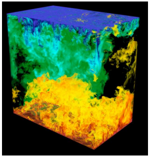
$$\boxed{\Omega_c \frac{d\mathbf{u}_c}{dt} + \mathsf{C}\left(\mathbf{u}_s\right)\mathbf{u}_c = \mathsf{D}\mathbf{u}_c - \mathsf{G}_c\mathbf{p}_c; \quad \mathsf{M}_c\mathbf{u}_c = \mathbf{0}_c}$$

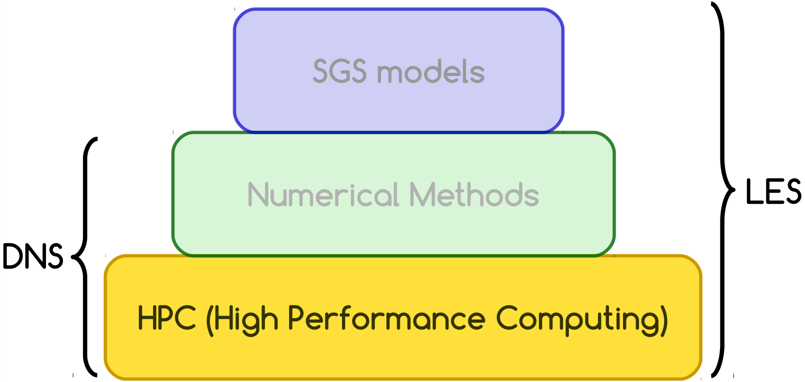
In <u>collocated meshes</u>

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



HPC on modern supercomputers

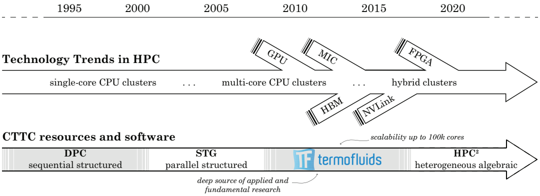




HPC on modern supercomputers

Research question #3:

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



[4] 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

[5] À.Alsalti, X.Álvarez, F.X.Trias, A.Oliva. *Exploiting spatial symmetries for solving Poisson's equation* **Journal of Computational Physics**, 486:112133, 2023.

HPC on modern supercomputers

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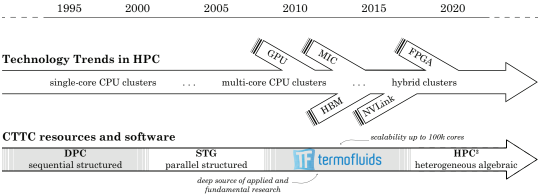

HPC^2: portable, algebra-based framework for heterogeneous computing is being developed[4]. Traditional stencil-based data and sweeps are replaced by algebraic structures (sparse matrices and vectors) and kernels. `SpMM`-based strategies to increase the arithmetic intensity are under development[5].

[4] 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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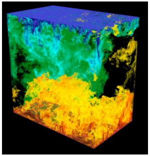
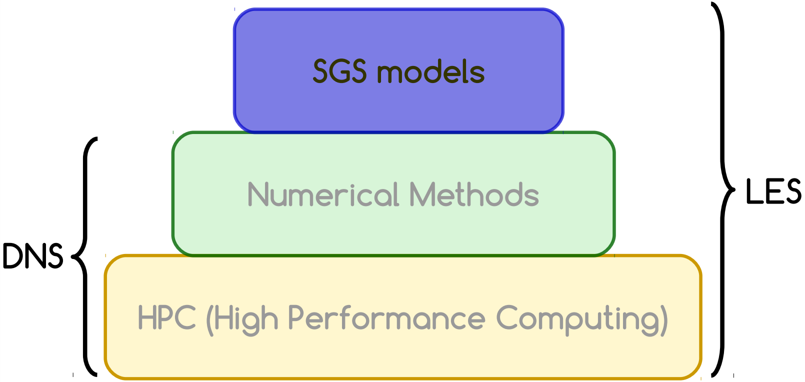
LES of RBC




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

Problems to model the SGS heat flux[6]

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

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

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

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

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

[6] 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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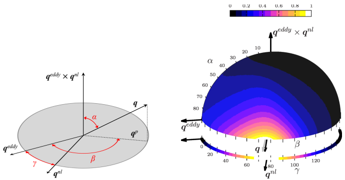

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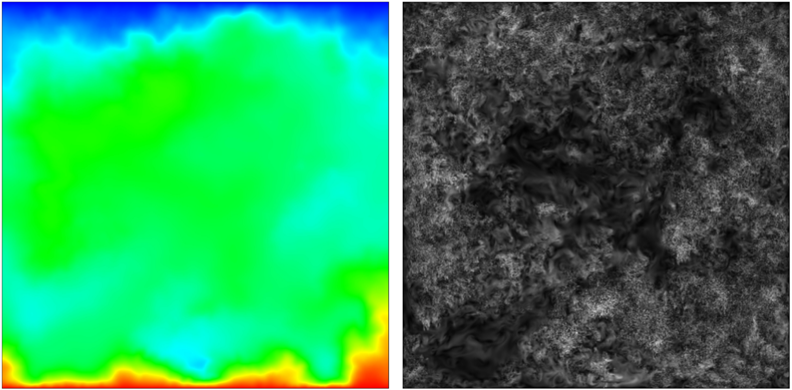

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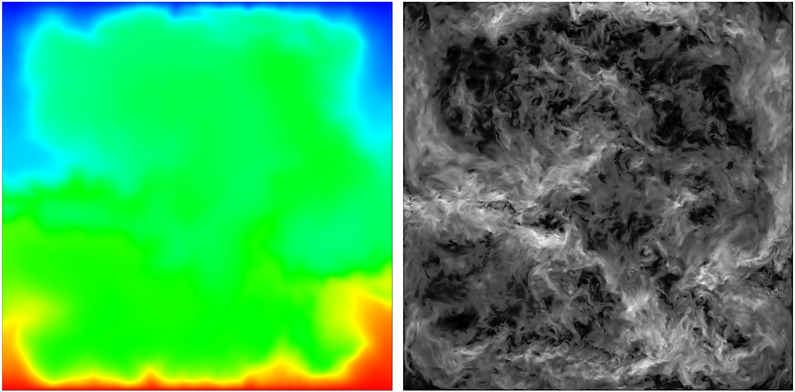

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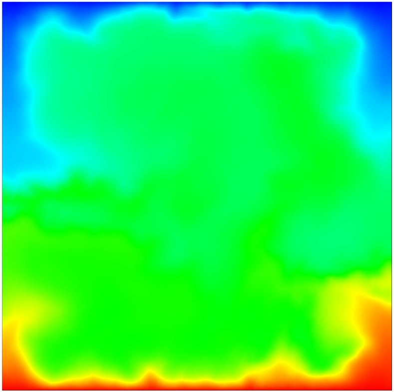

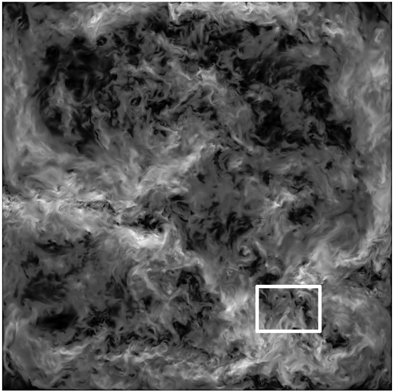

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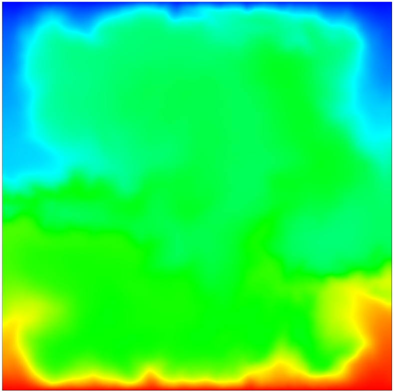

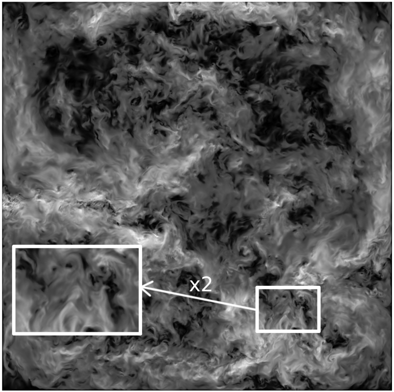

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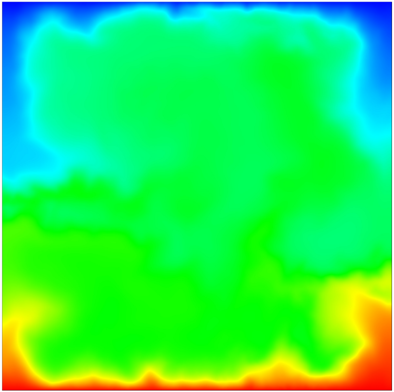

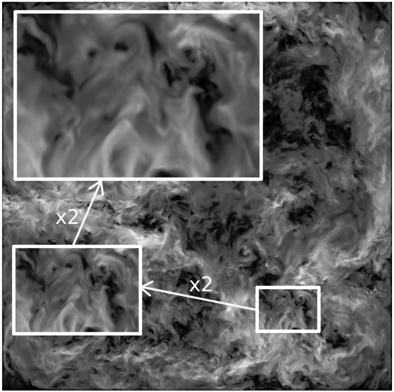

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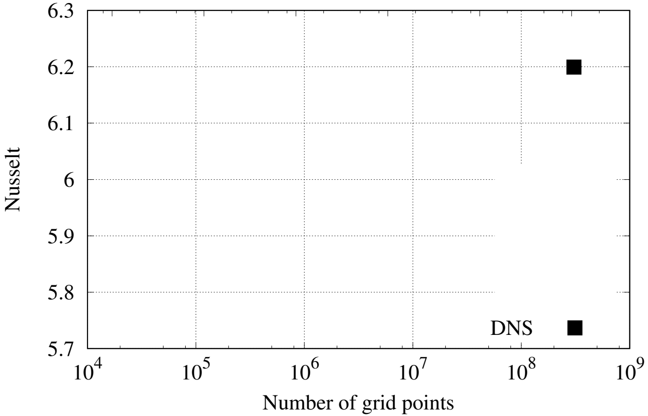

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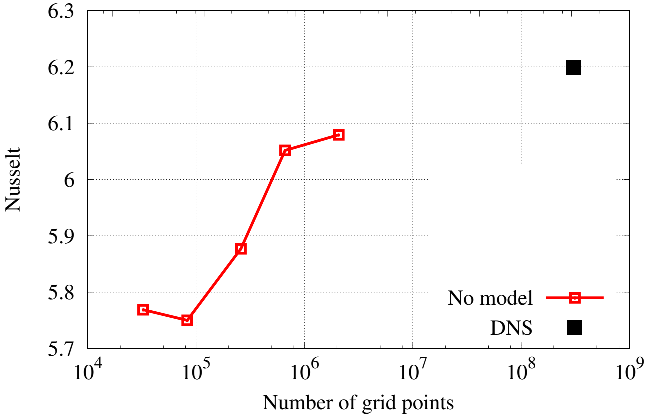

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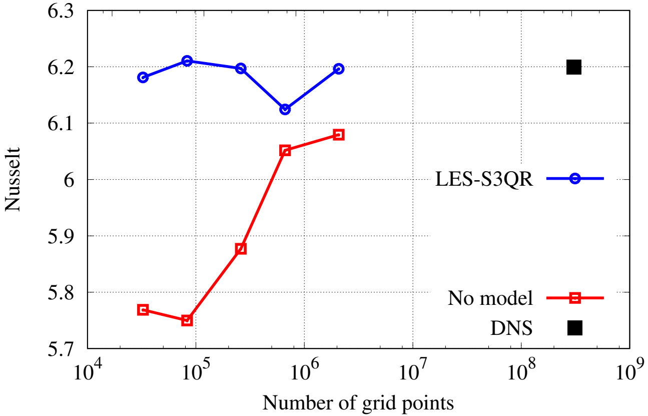

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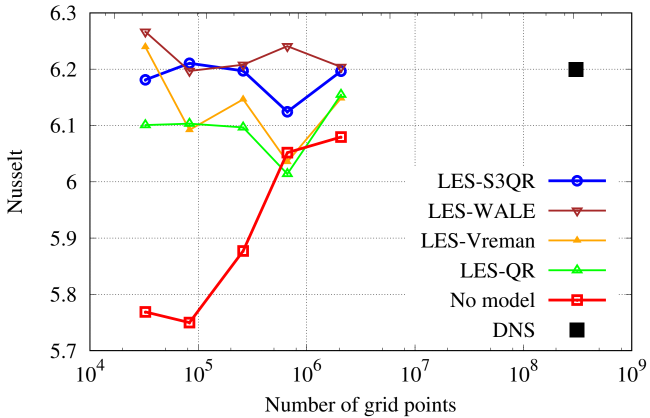

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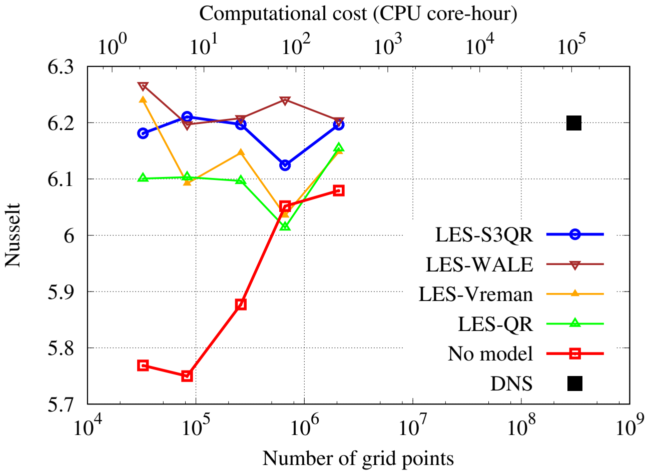

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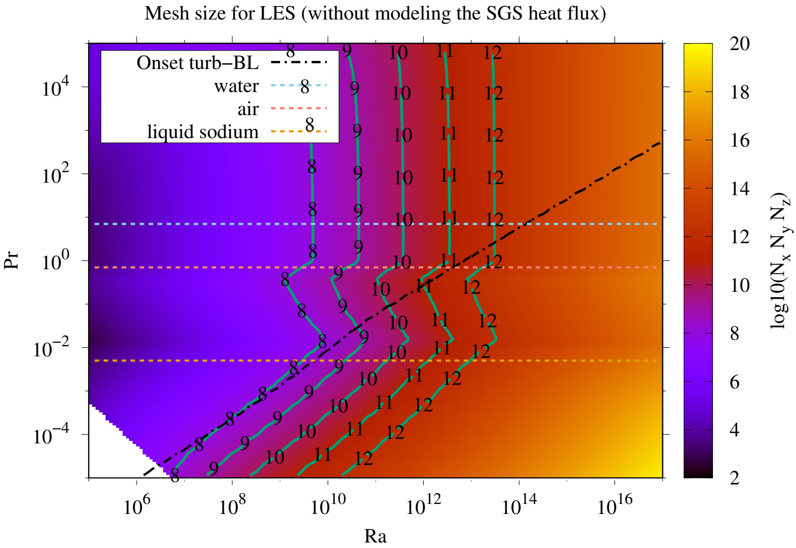

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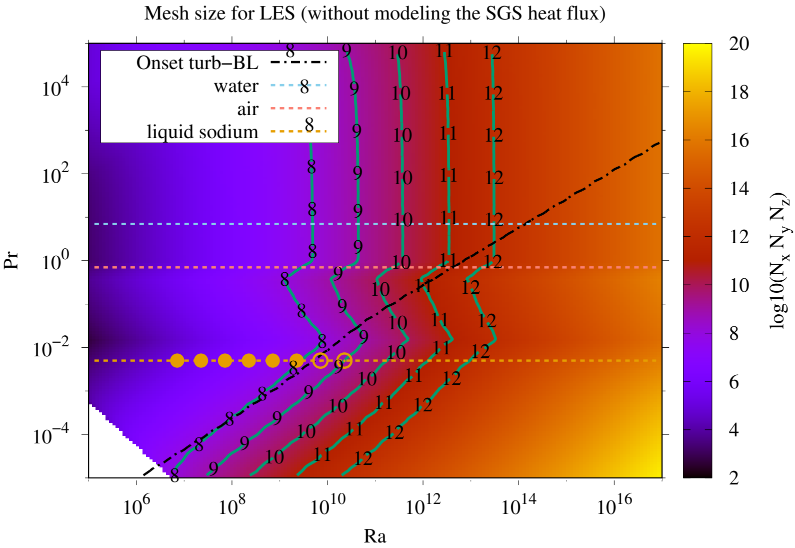

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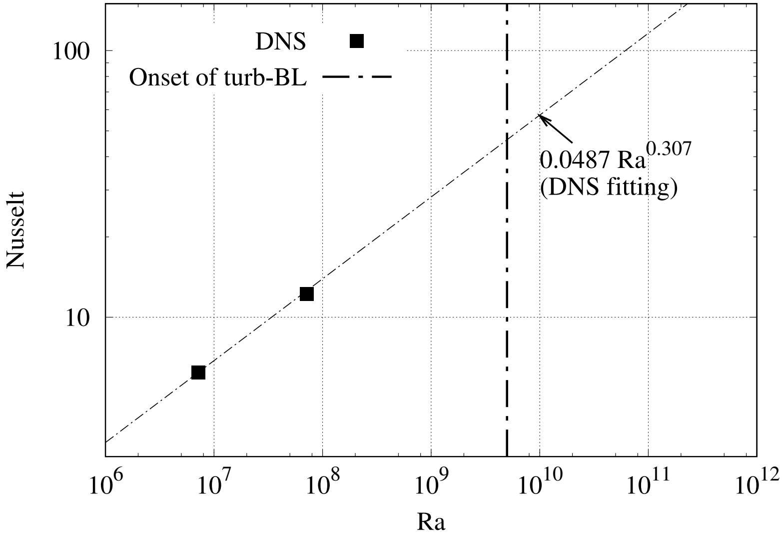

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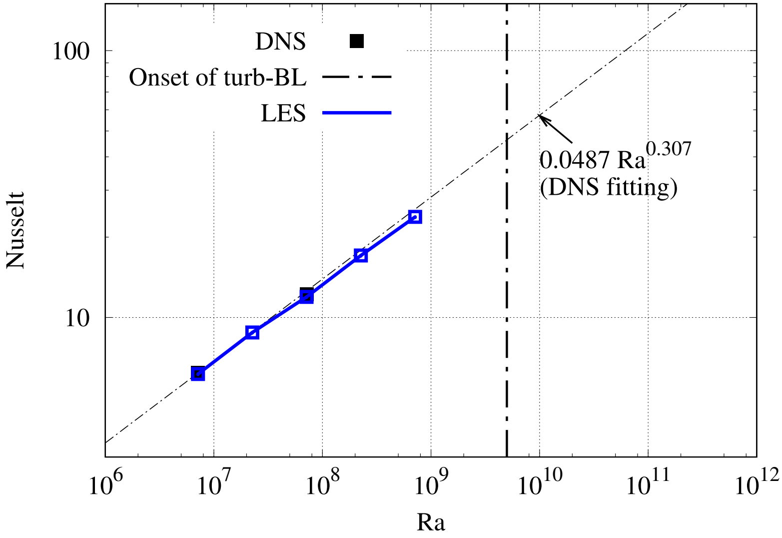

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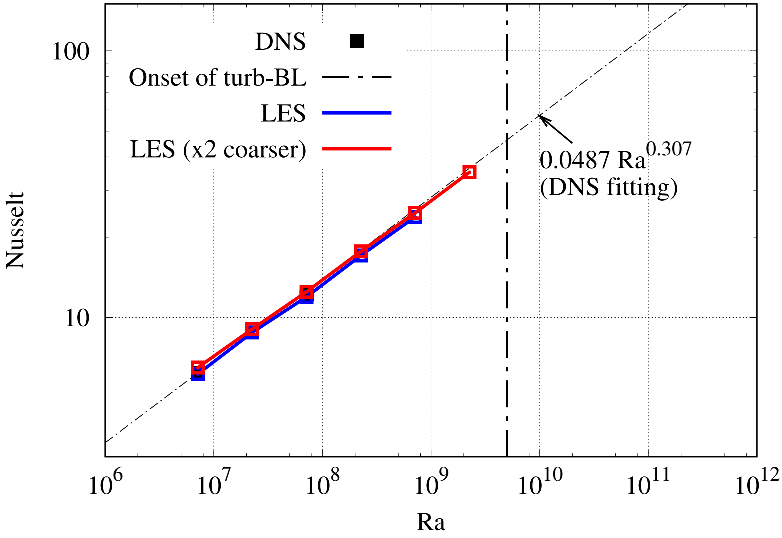

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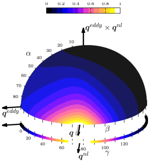

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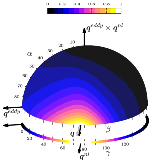

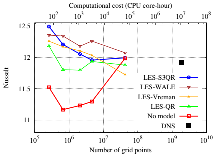

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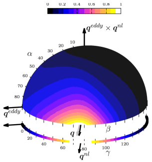

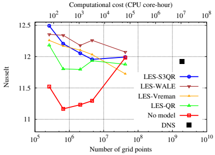

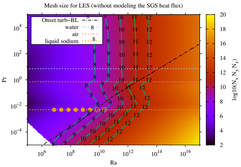

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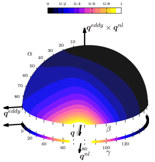
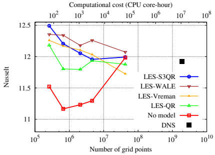
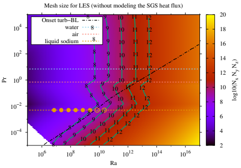




On-going research:

- 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