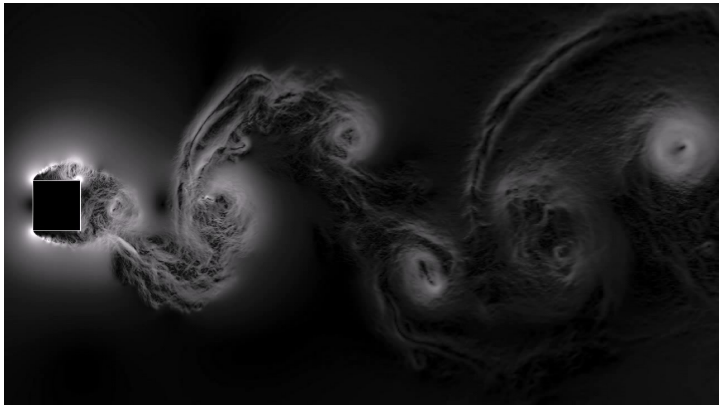
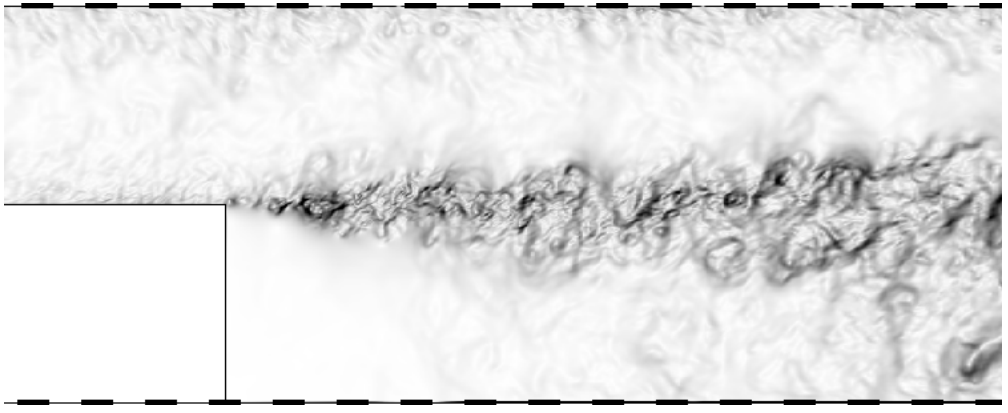
Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

Preserving symmetries on unstructured grids

F.Xavier Trias

Heat and Mass Transfer Technological Center, Technical University of Catalonia (UPC)



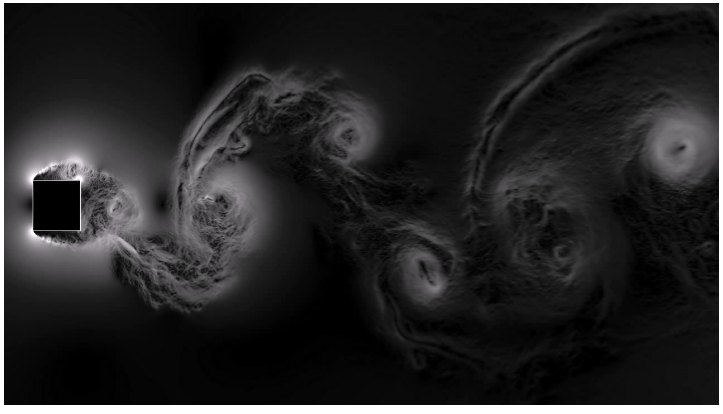


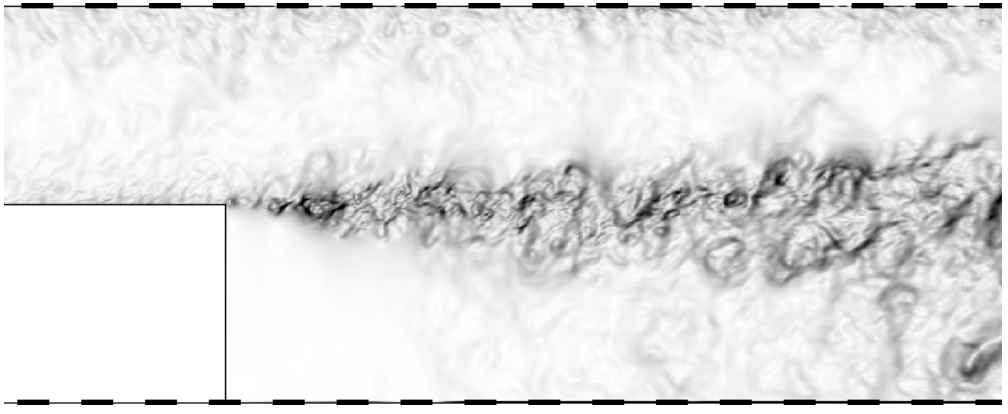
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Preserving symmetries on unstructured grids: paving the way for DNS and LES on complex geometries

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Contents

1. Background
2. Preserving symmetries at discrete level
3. LES of RBC
4. Portability and beyond
5. Conclusions

About myself...

Professional...

- Current position (since 2018): **Associate Professor** at UPC
- Previous positions: PostDoc at University of Groningen (2007-2009) and UPC (2010-2013), and *Ramón y Cajal* Senior Researcher at UPC (2013-2018).
- My **research** focus is on fluid mechanics, turbulence modeling, physics and numerics of complex flows, applied mathematics and numerical methods.
- Some numbers: 51 papers, 165 conferences, 10 PhD's+5 (on-going)
- Stays and collaborations: Groningen (Netherlands), UCLA, KIAM (Russian Academy of Sciences), Stanford, Tsinghua (China), TokioTech (Japan), Napoli (Italy), CWI (Netherlands),...
- More info: www.fxtrias.com

About myself...

... and more personal stuff

- My complete name: Francesc Xavier Trias Miquel
- Born in Barcelona
- My mother tongue is Catalan. I also speak Spanish at native level.
- Hobbies? I like my work but also sports. Most practiced ones are running and football:





Groningen (2009?)



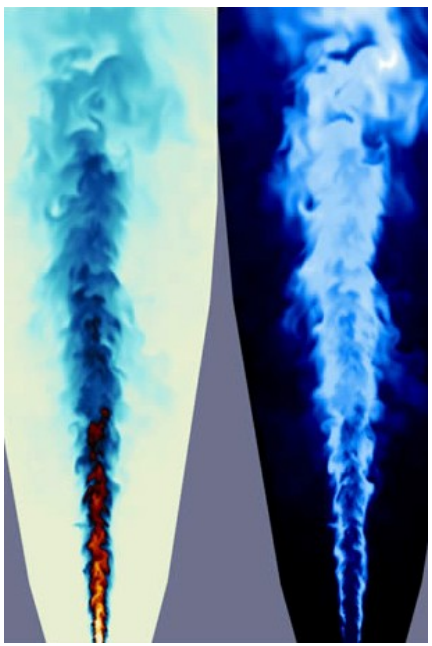


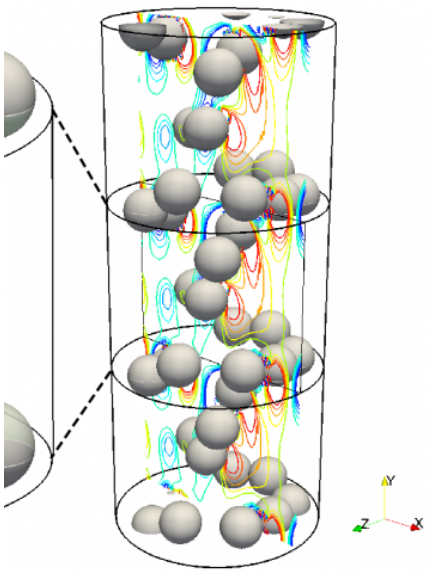
Barcelona (2019)

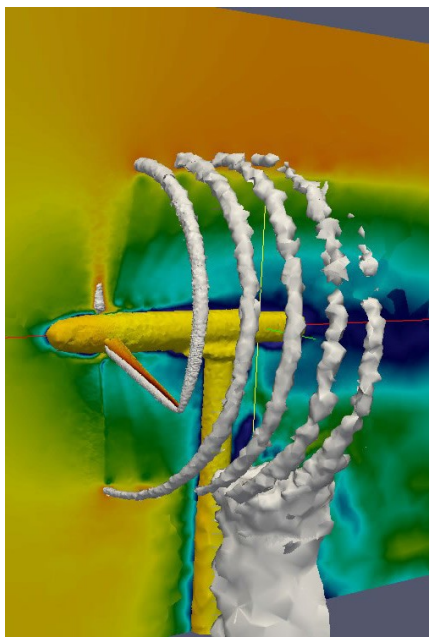
The CTTC research group

Heat and Mass Transfer Technological Center (Catalan: *Centre Tecnològic de Transferència de Calor*) has more than 30 years experience on CFD:

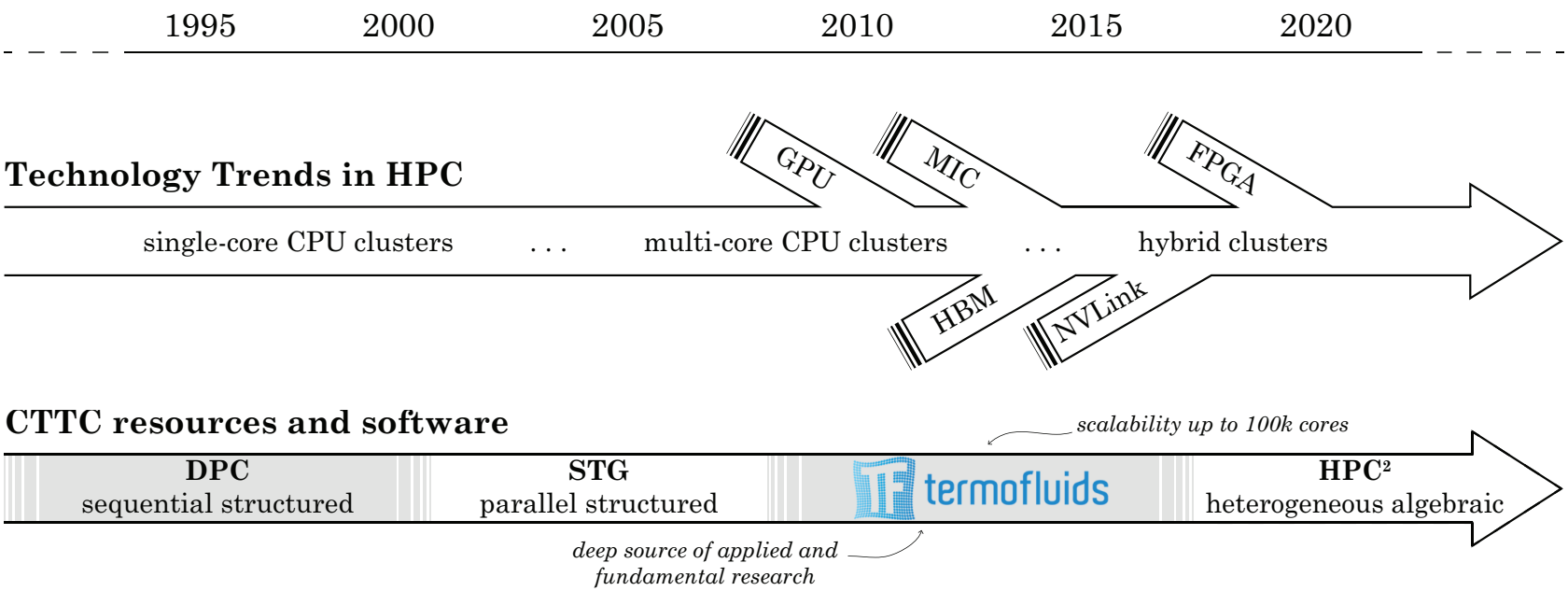
- **Fundamental research** on numerical methods, fluid dynamics and heat and mass transfer phenomena.
- **Applied research** on thermal and fluid dynamic optimization of thermal system and equipment.







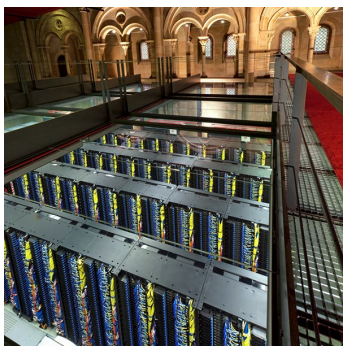
CTTC's historical background in HPC

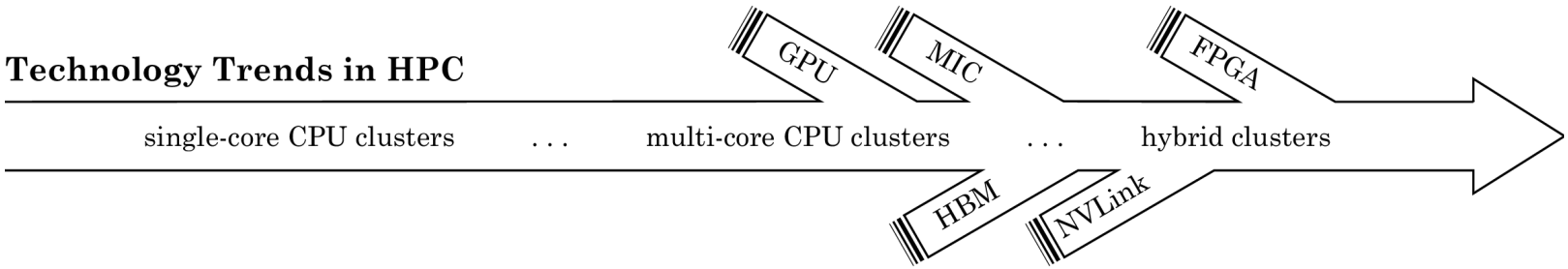


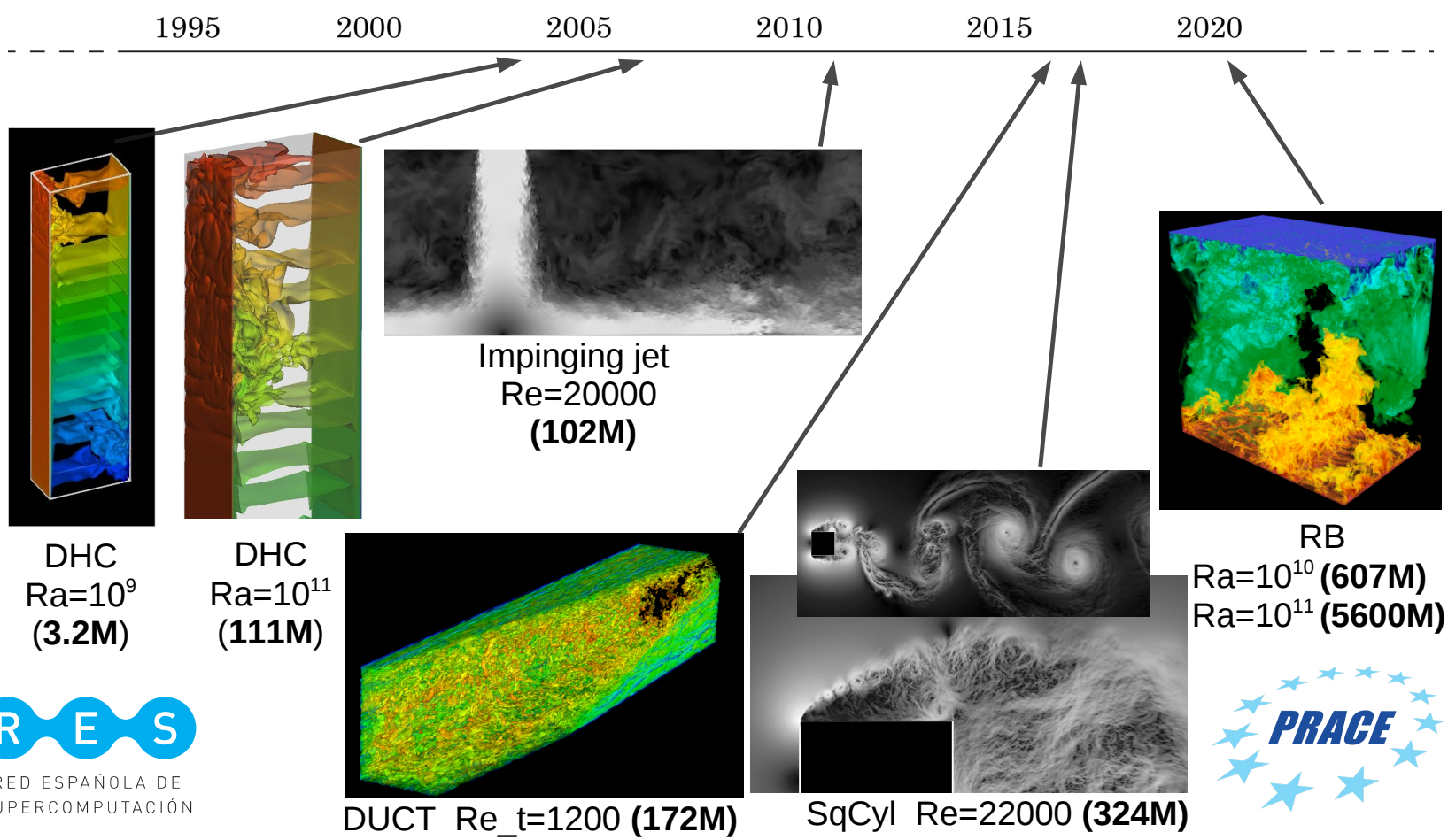




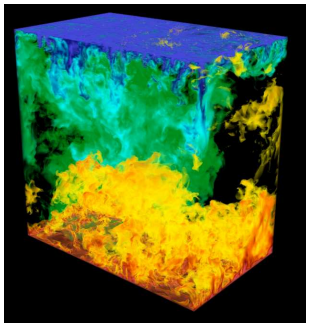





Technology Trends in HPC
GPU
MIC
FPGA
single-core CPU clusters
. . .
multi-core CPU clusters
. . .
hybrid clusters
HBM
NVLink

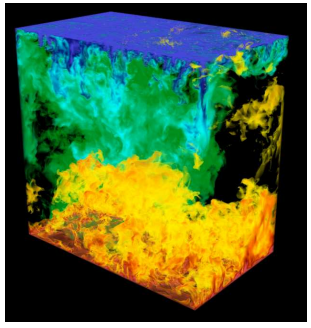

1995
2000
2005
2010
2015
2020
DHC
Ra=10^9
(3.2M)
DHC
Ra=10^11
(111M)
Impinging jet
Re=20000
(102M)
RB
Ra=10^10 (607M)
Ra=10^11 (5600M)
DUCT Re_t=1200 (172M)
SqCyl Re=22000 (324M)
RED ESPAÑOLA DE SUPERCOMPUTACIÓN
PRACE

General motivation: (very) large-scale DNS/LES



DNS

General motivation: (very) large-scale DNS/LES





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

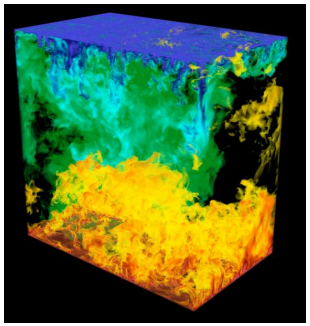
PRACE



DNS

HPC (High Performance Computing)

General motivation: (very) large-scale DNS/LES



How to properly discretize NS?

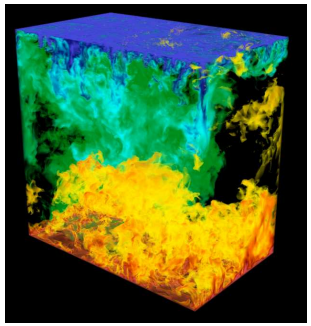
DNS

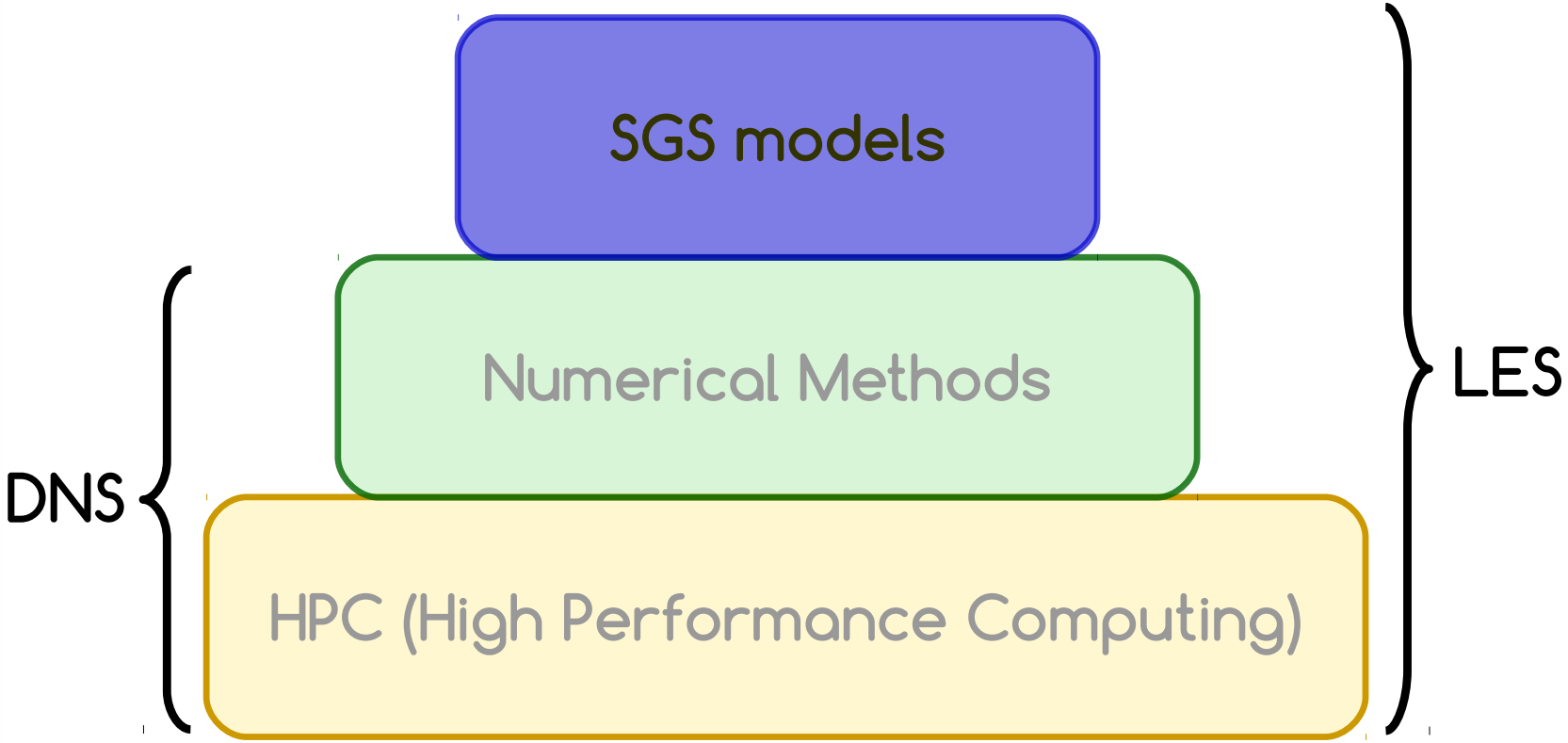
Numerical Methods

HPC (High Performance Computing)

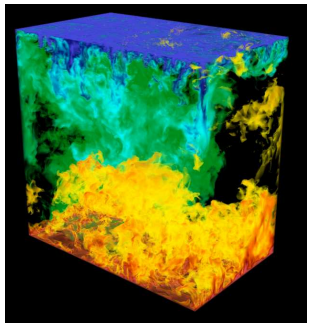
General motivation: (very) large-scale DNS/LES

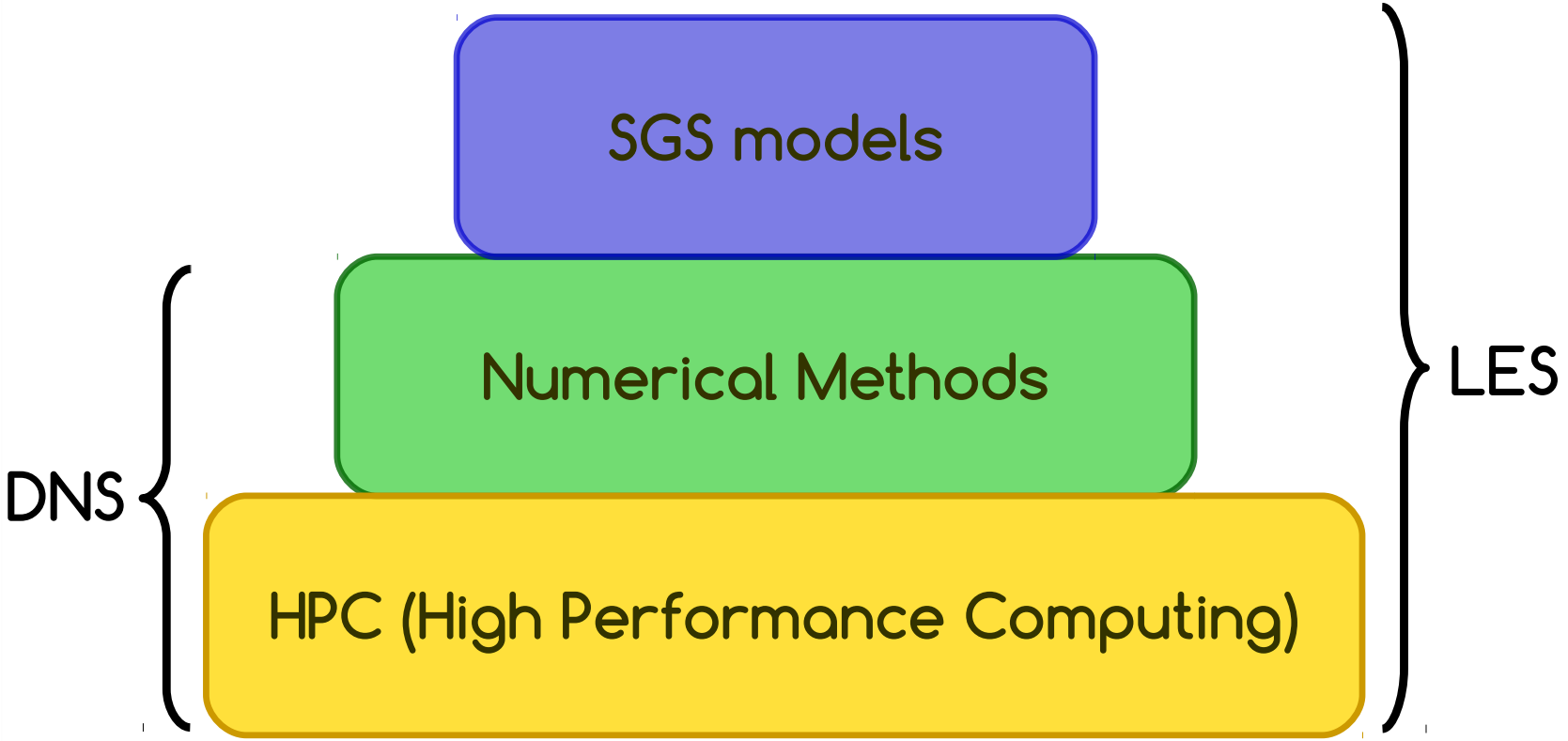
How to properly model SGS?



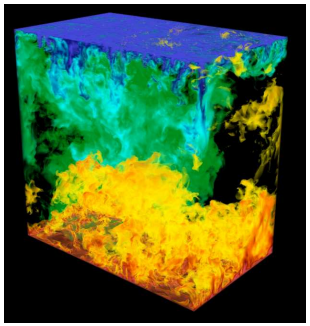


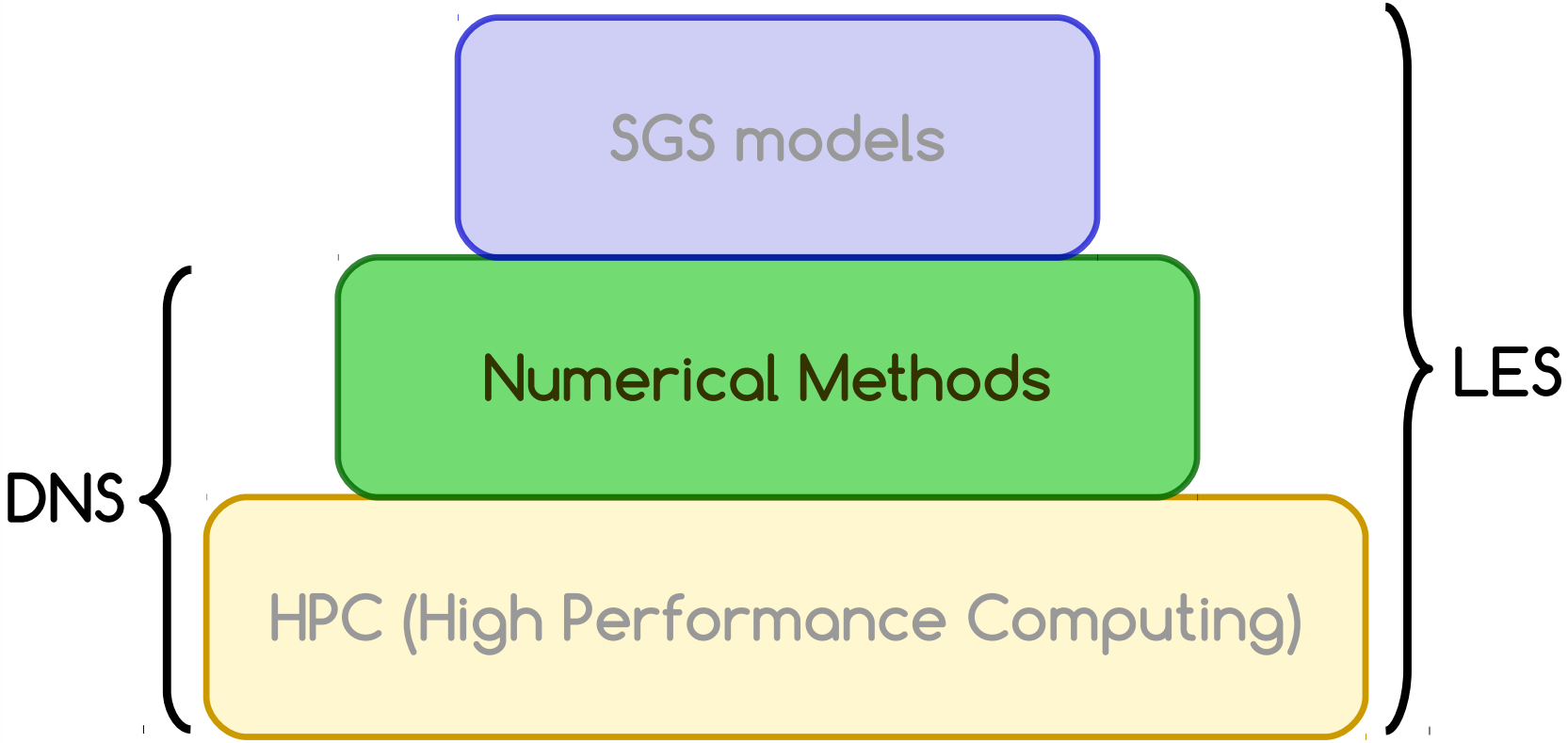
General motivation: (very) large-scale DNS/LES





Numerical methods for DNS/LES

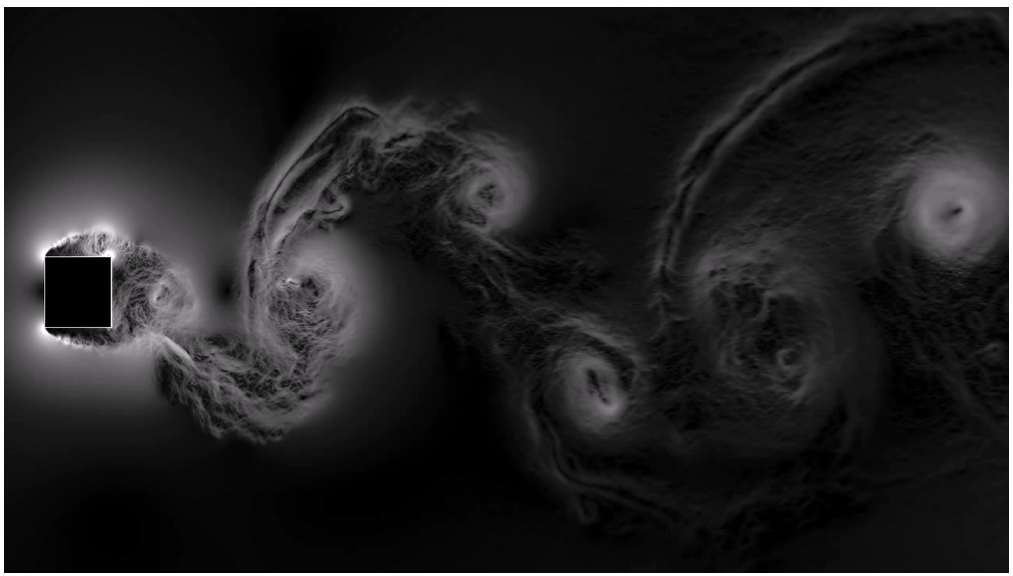


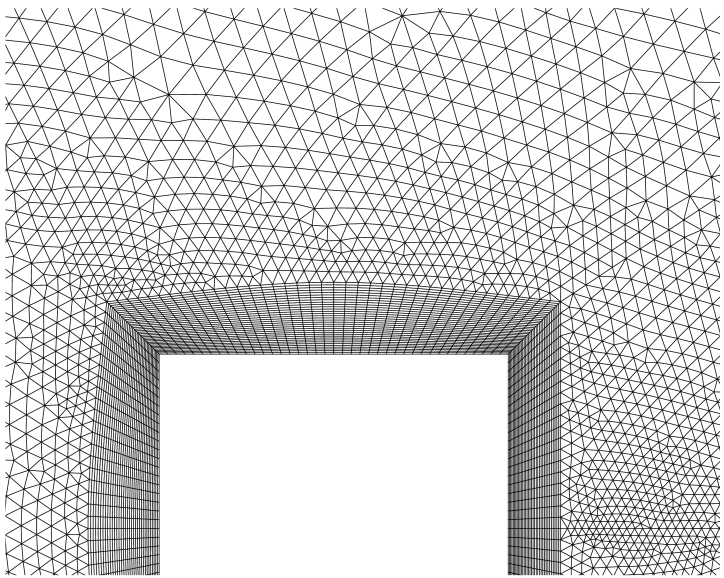


Numerical methods for DNS/LES

Research question #1:

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





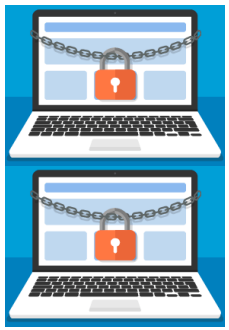
DNS[1] of the turbulent flow around a square cylinder at $Re = 22000$

[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.

Motivation

Frequently used general purpose CFD codes:

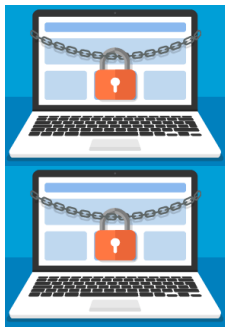
- STAR-CCM+
- ANSYS-FLUENT
- Code-Saturne
- OpenFOAM



Motivation

Frequently used general purpose CFD codes:

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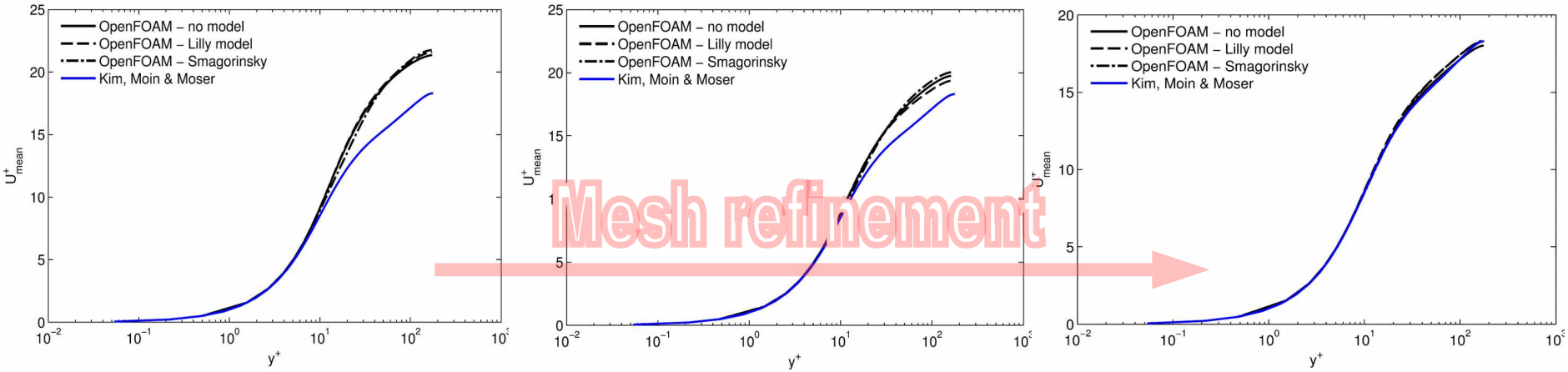


Main common characteristics of LES in such codes:

- **Unstructured finite volume** method, **collocated** grid
- Second-order spatial and temporal discretisation
- Eddy-viscosity type LES models

Motivation

OpenFOAM® LES[3] results of a turbulent channel for at $Re_\tau = 180$



$13 \times 76 \times 20$

$\Delta x^+ = 90, \Delta y^+_{wall} = 0.5, \Delta z^+ = 30$

$19 \times 78 \times 28$

$\Delta x^+ = 60, \Delta y^+_{wall} = 0.5, \Delta z^+ = 20$

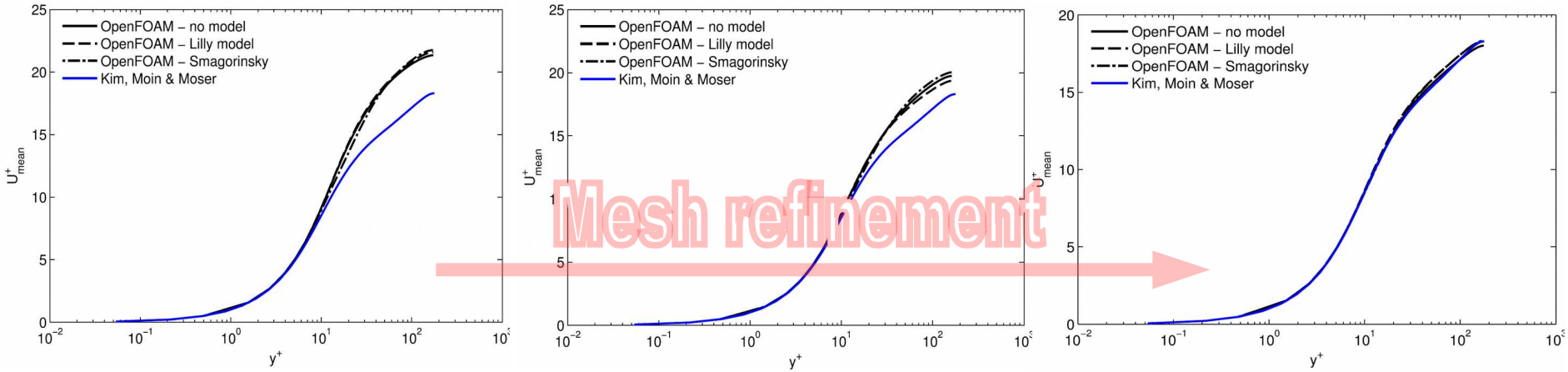
$38 \times 78 \times 57$

$\Delta x^+ = 30, \Delta y^+_{wall} = 0.5, \Delta z^+ = 10$

[3] 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.

Motivation

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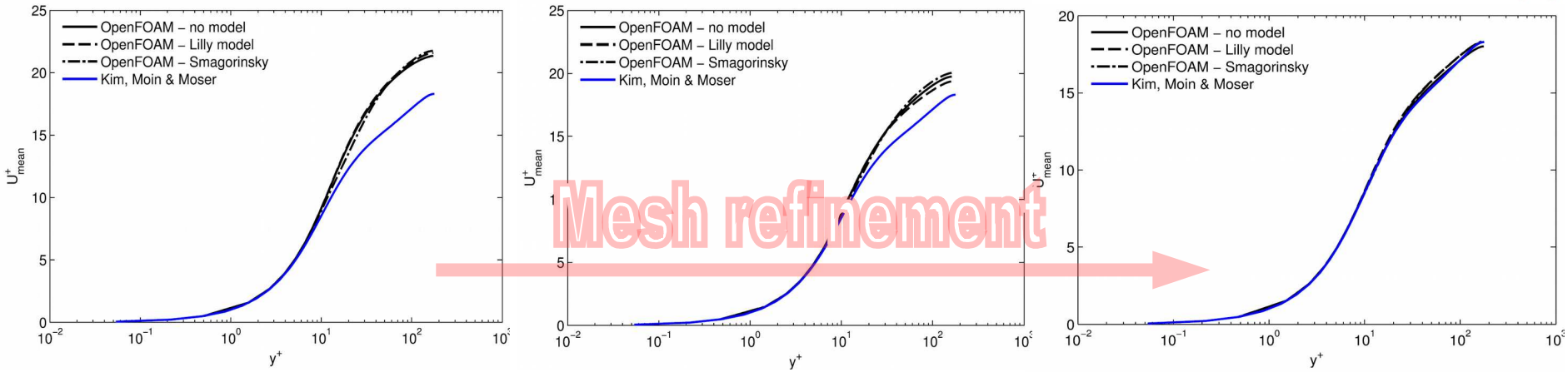
$\Delta x^+ = 30, \Delta y^+_{wall} = 0.5, \Delta z^+ = 10$

- Are LES results are merit of the SGS model?

[3] 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.

Motivation

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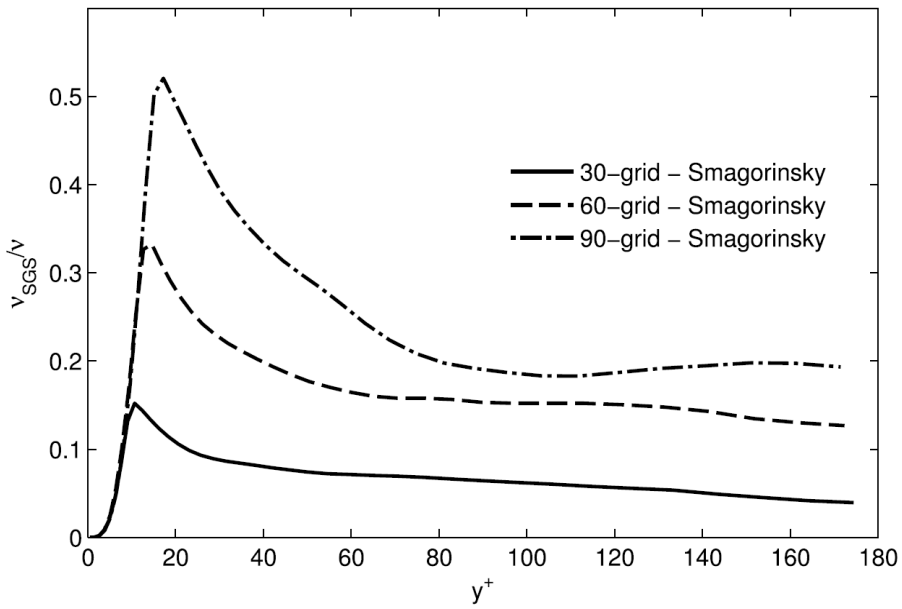
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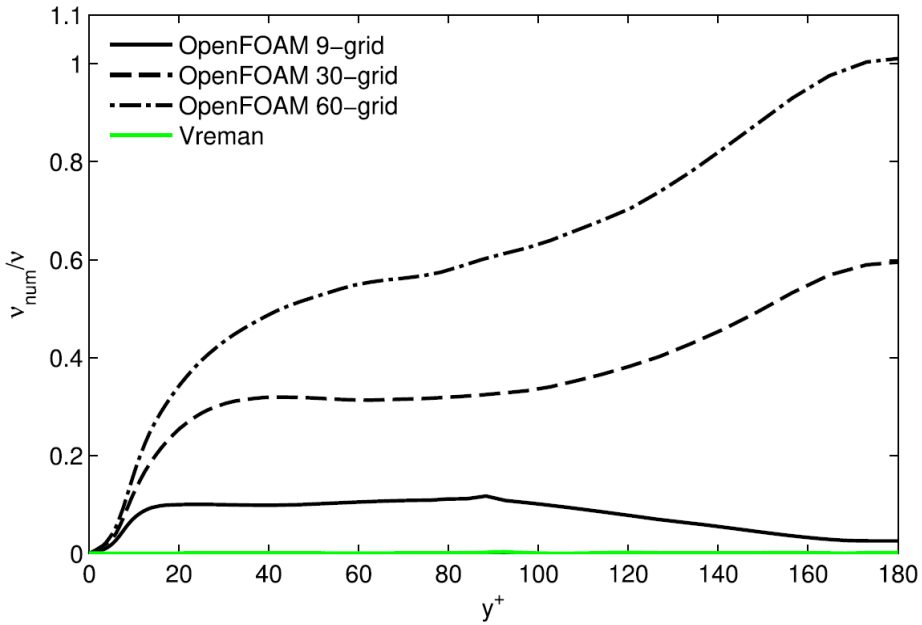
- Are LES results are merit of the SGS model? Apparently **NOT**!!! ✗

[3] 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.

Motivation

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



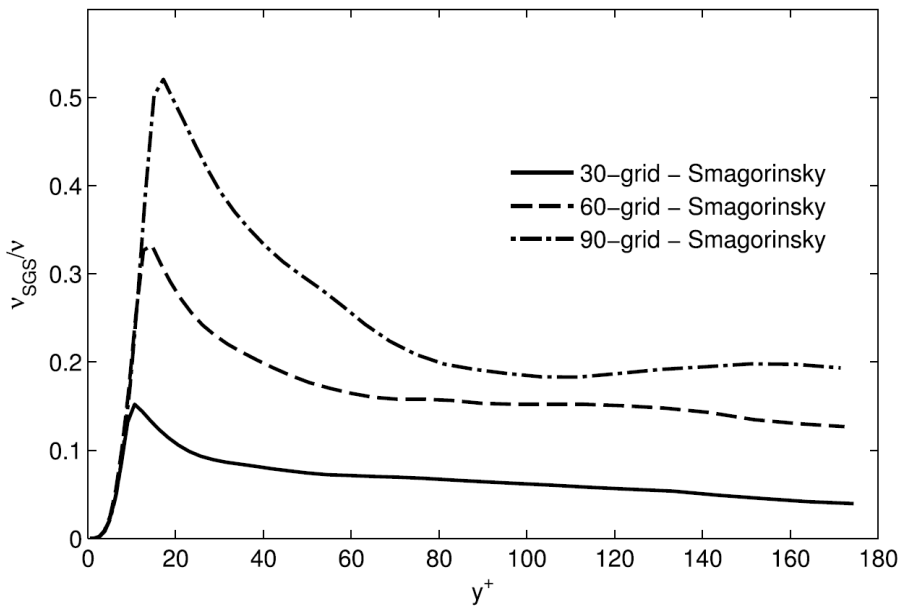


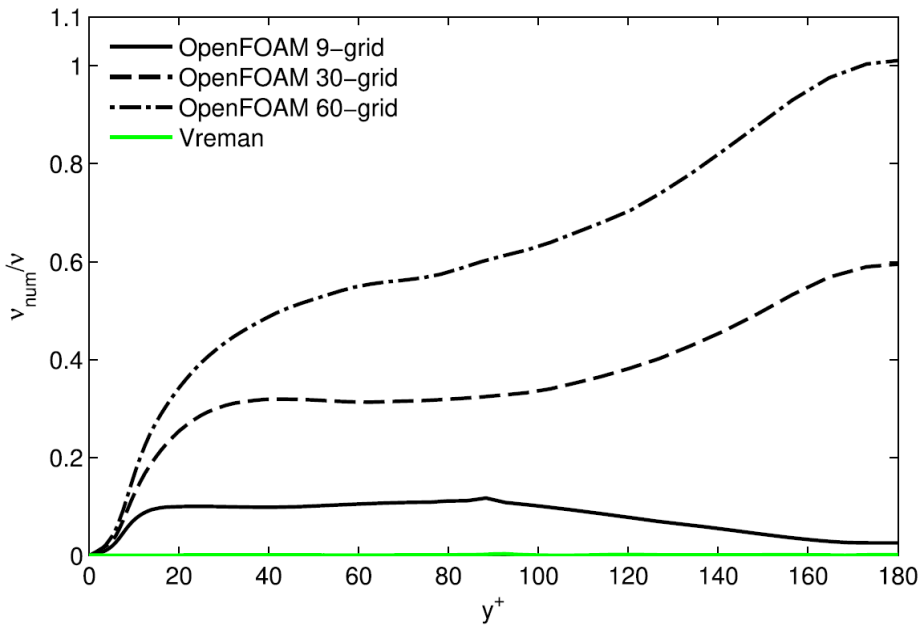
$$\nu_{num} \neq 0$$

[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.

Motivation

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





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

[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.

Symmetry-preserving discretization

Continuous

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

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

Symmetry-preserving discretization

Continuous

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

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

Discrete

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

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

Symmetry-preserving discretization

Continuous

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

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

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

Discrete

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

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

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

Symmetry-preserving discretization

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

Symmetry-preserving discretization

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

Symmetry-preserving discretization

Continuous

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

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

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

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

$$\left\langle \nabla \cdot \boldsymbol{a}, \varphi \right\rangle = -\left\langle \boldsymbol{a}, \nabla \varphi \right\rangle$$

$$\left\langle \nabla^2 \boldsymbol{a}, \boldsymbol{b} \right\rangle = \left\langle \boldsymbol{a}, \nabla^2 \boldsymbol{b} \right\rangle$$

Discrete

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

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

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

$$\mathrm{C}\left(\boldsymbol{u}_h\right) = -\mathrm{C}^T\left(\boldsymbol{u}_h\right)$$

$$\Omega \mathrm{G} = -\mathrm{M}^T$$

$$\mathrm{D} = \mathrm{D}^T \qquad def -$$

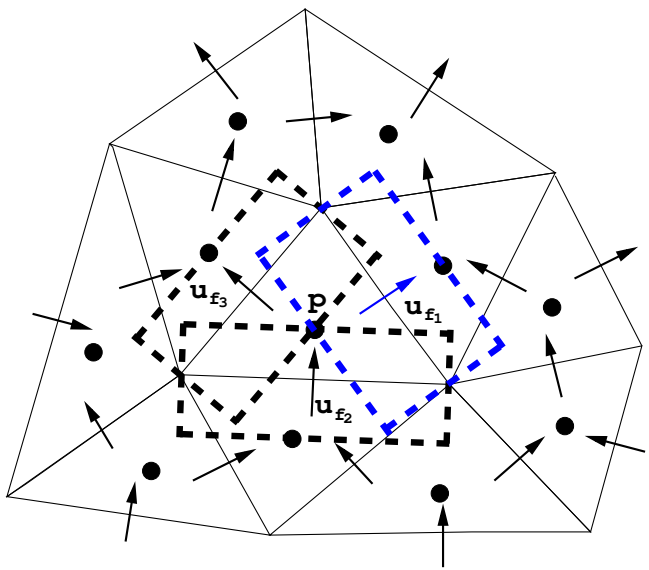
Why collocated arrangements are so popular?

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

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

In staggered meshes

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



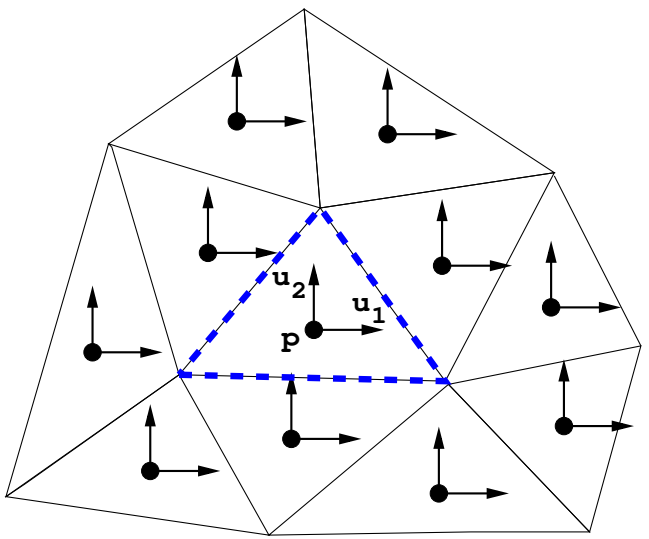
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In collocated meshes

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



Why collocated arrangements are so popular?

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

- STAR-CCM+ 




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- Code-Saturne 





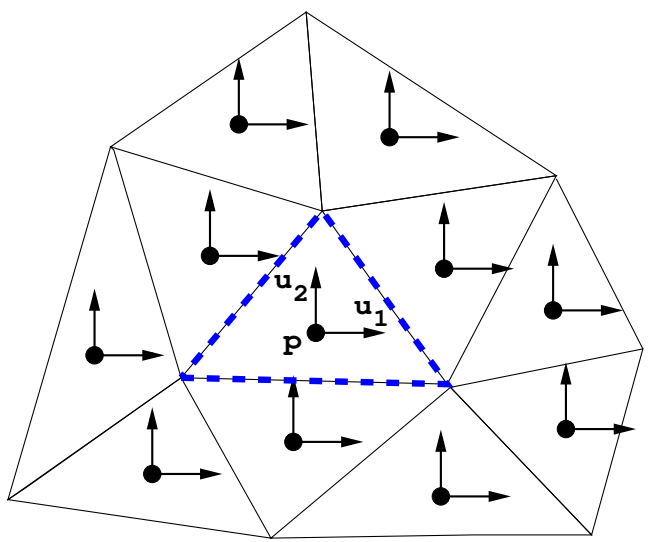
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Pressure-velocity coupling on collocated grids

A vicious circle that cannot be broken...

In summary[5]:

- Mass: $\mathrm{M}\Gamma_{c\to s}\boldsymbol{u}_c = \mathrm{M}\Gamma_{c\to s}\boldsymbol{u}_c - \mathrm{L}_c\mathrm{L}^{-1}\,\mathrm{M}\Gamma_{c\to s}\boldsymbol{u}_c \approx \mathbf{0}_c$ ✗
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[5] 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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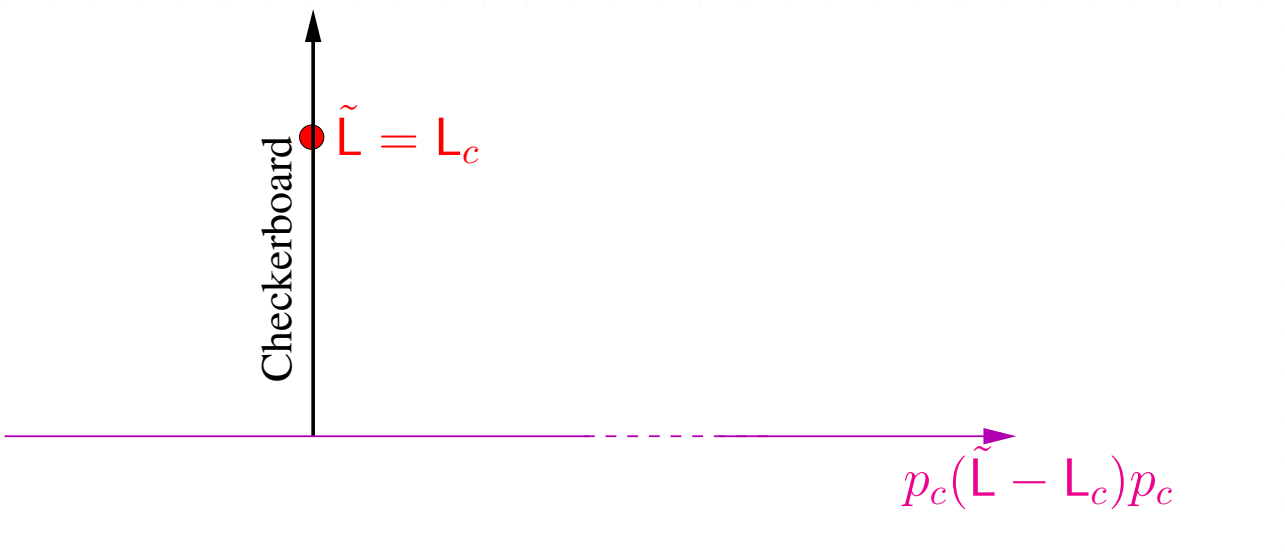
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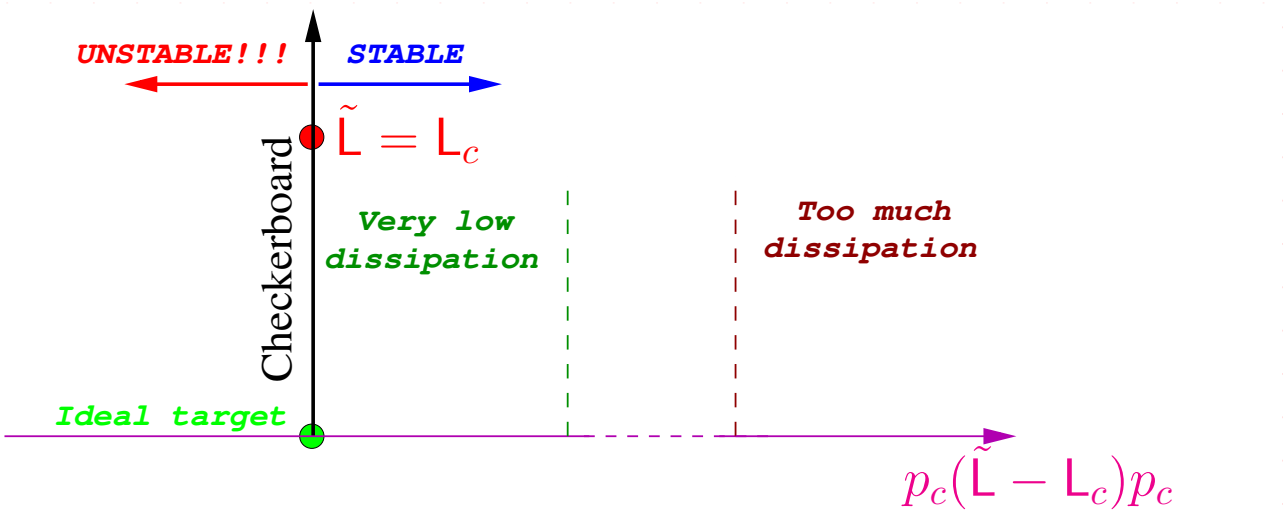
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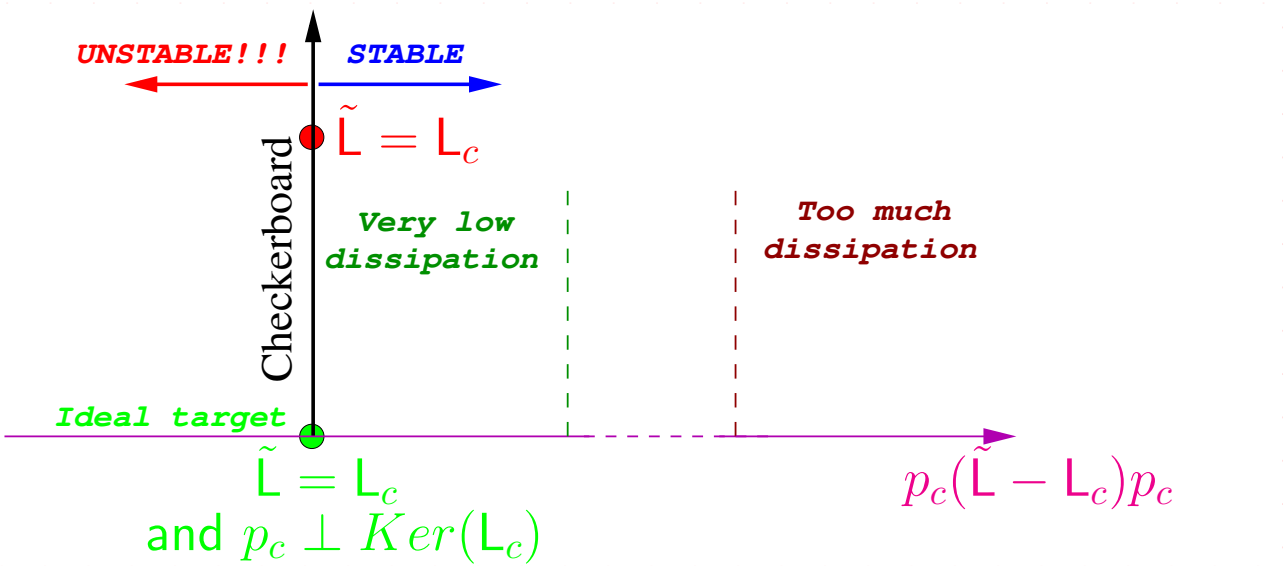
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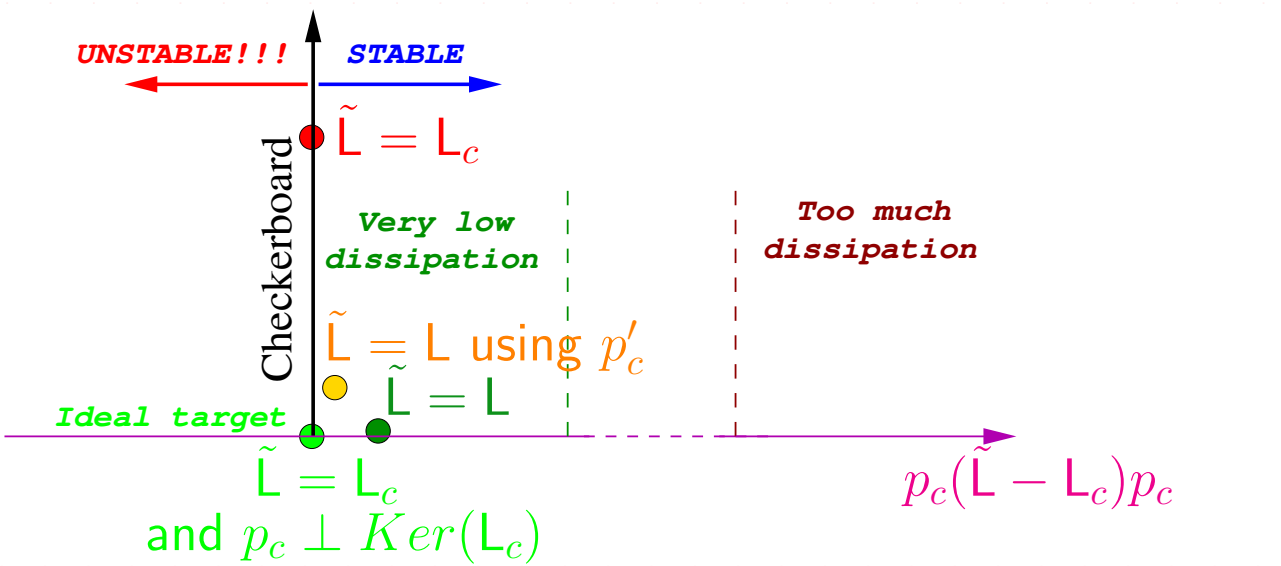
[5] Shashank, J.Larsson, G.Iaccarino. *A co-located incompressible Navier-Stokes solver with exact mass, momentum and kinetic energy conservation in the inviscid limit*, **Journal of Computational Physics**, 229: 4425-4430,2010.

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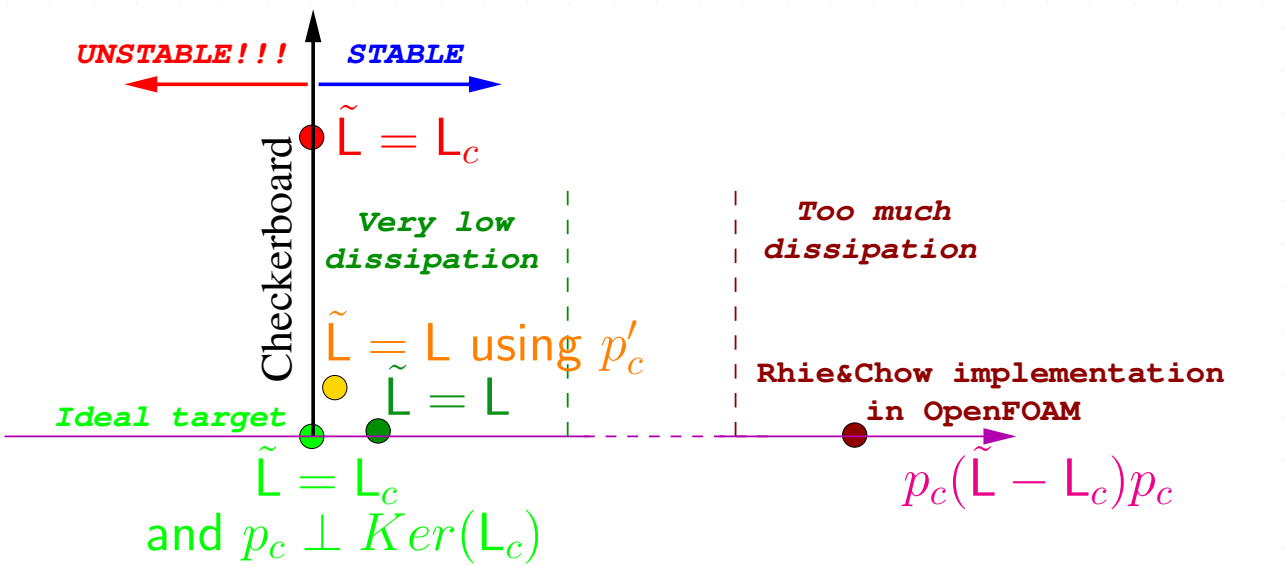
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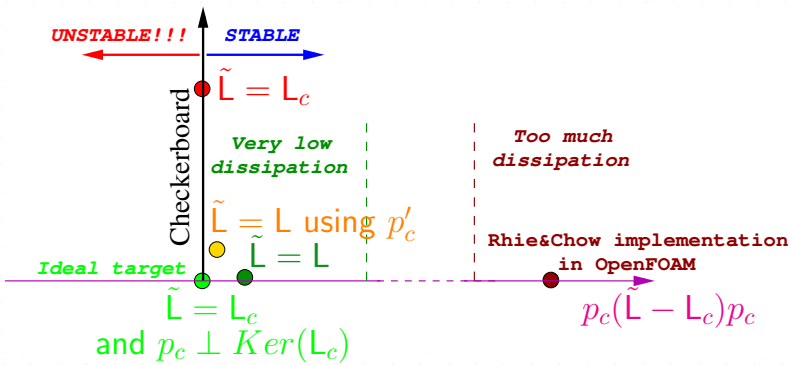
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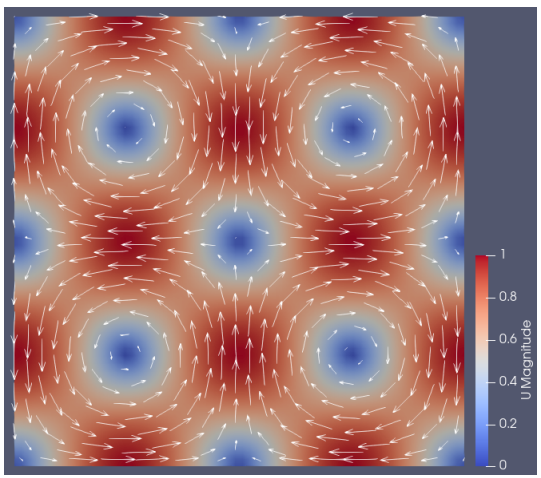


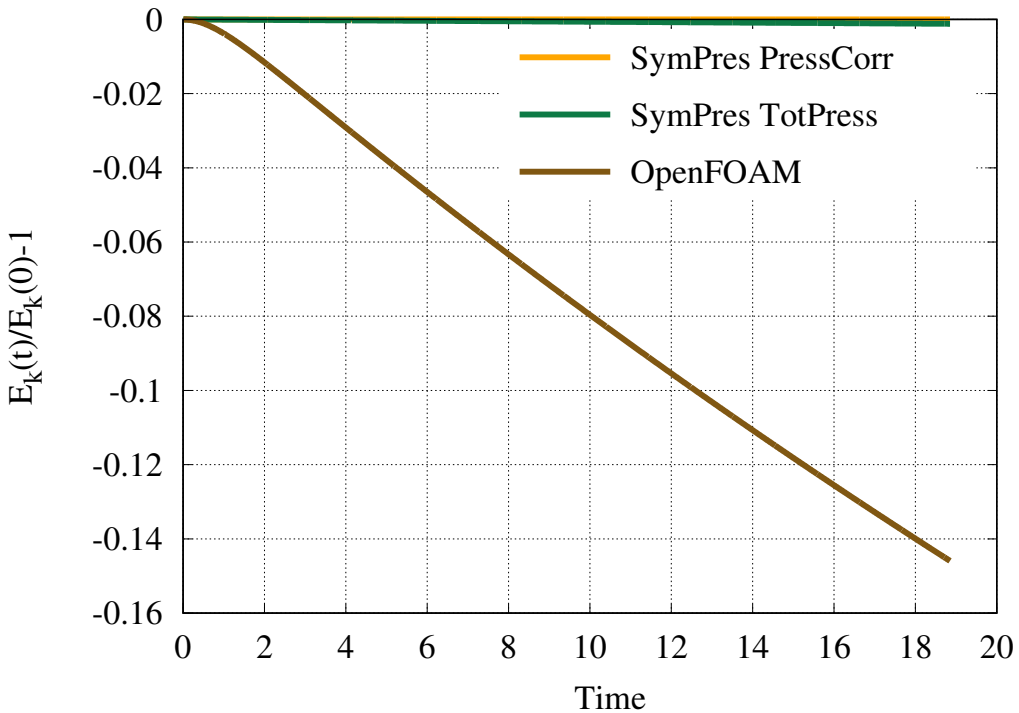
[5] E.Komen, J.A.Hopman, E.M.A.Frederix, F.X.Trias, R.W.C.P.Verstappen. "A symmetry-preserving second-order time-accurate PISO-based method". **Computers & Fluids**, 225:104979, 2021. (github.com/janneshopman)

Pressure-velocity coupling on collocated grids

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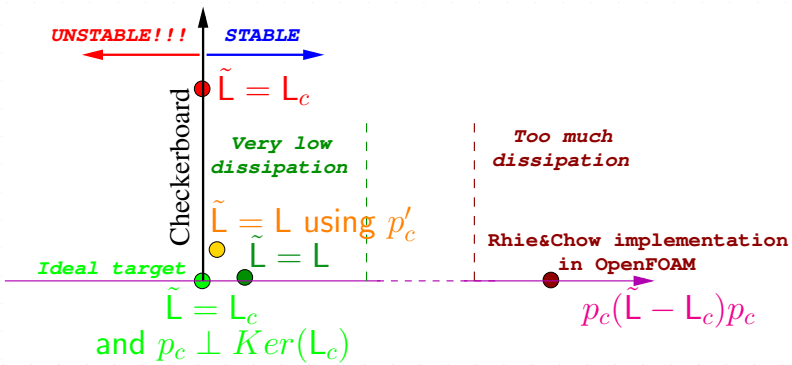


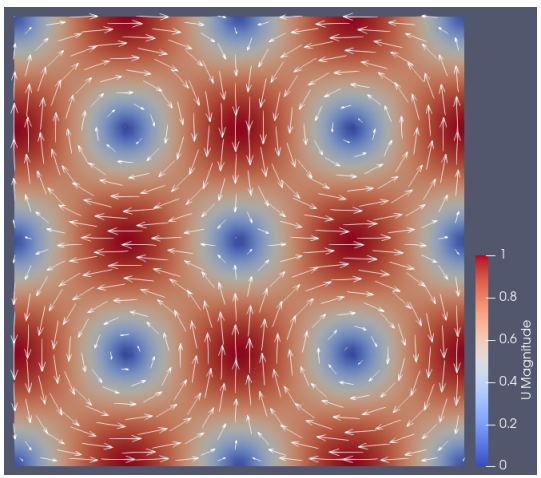
Results for an inviscid Taylor-Green vortex[6]

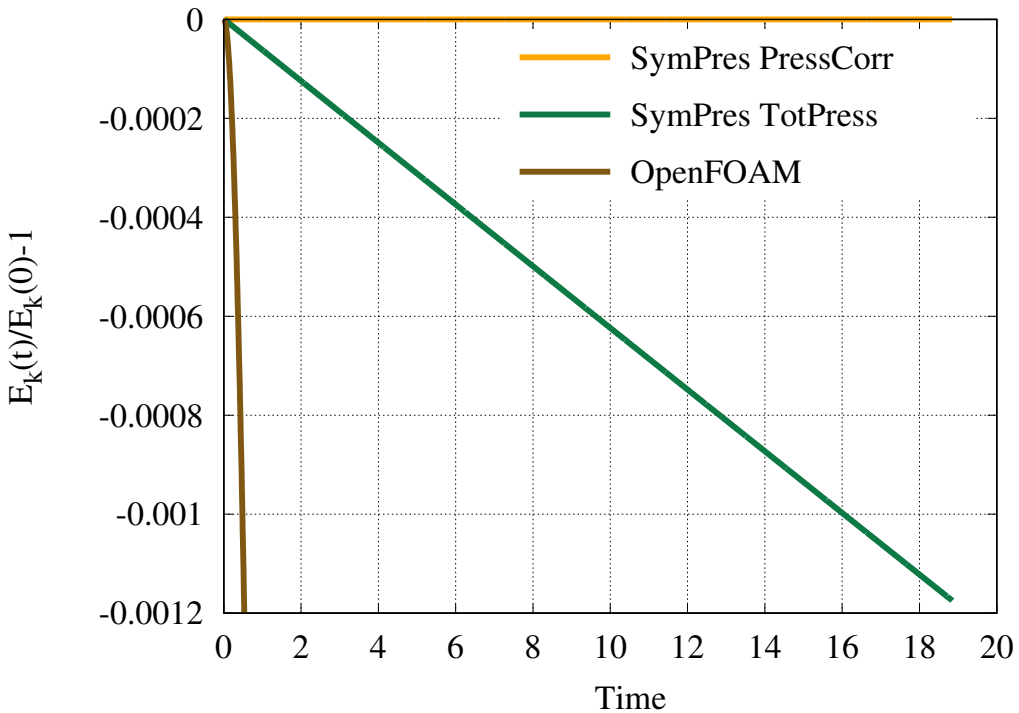
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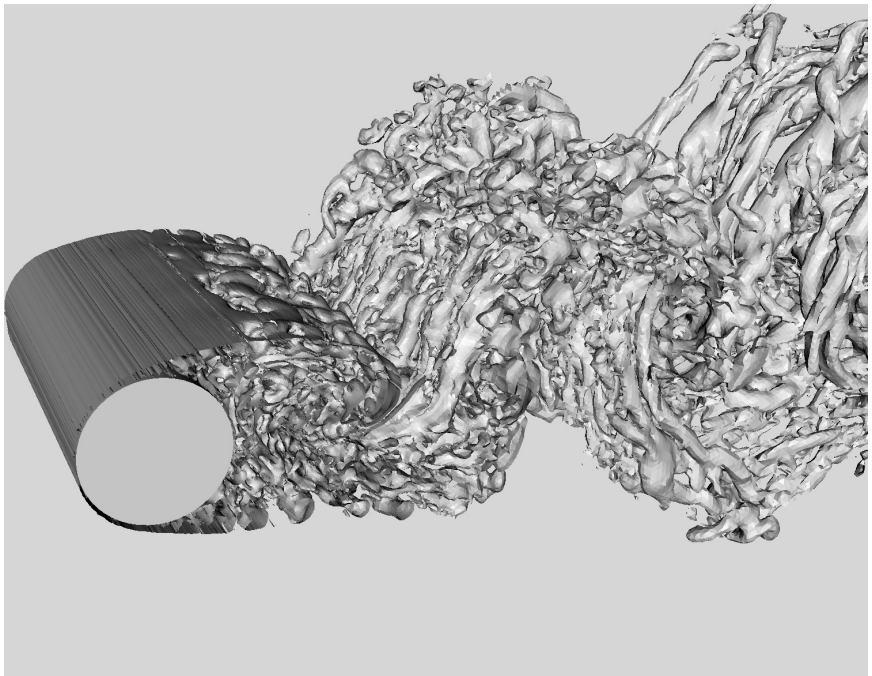
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Pressure-velocity coupling on collocated grids

Examples of simulations

Despite these inherent limitations, symmetry-preserving collocated formulation has been successfully used for DNS/LES simulations[7]:



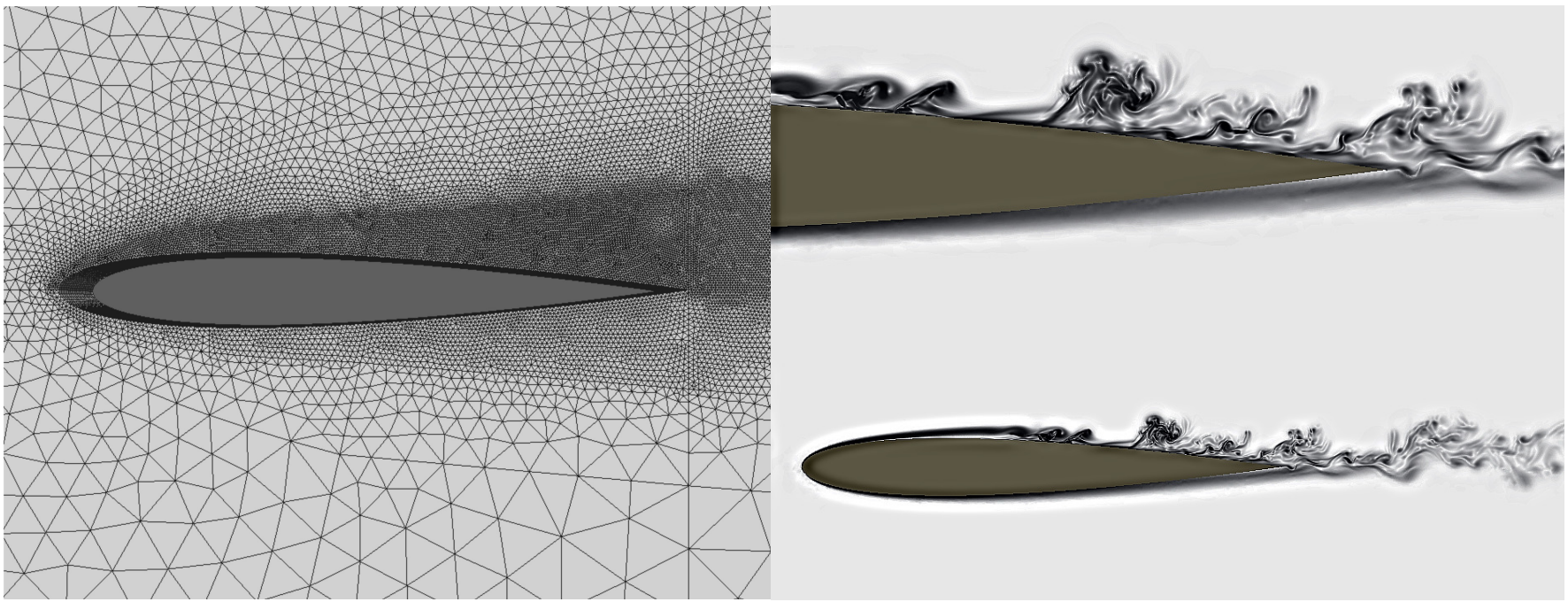


[7] R.Borrell, O.Lehmkuhl, F.X.Trias, A.Oliva. *Parallel Direct Poisson solver for discretizations with one Fourier diagonalizable direction*. **Journal of Computational Physics**, 230:4723-4741, 2011.

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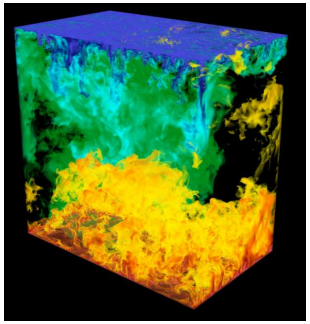
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LES of RBC



SGS models

Numerical Methods

HPC (High Performance Computing)

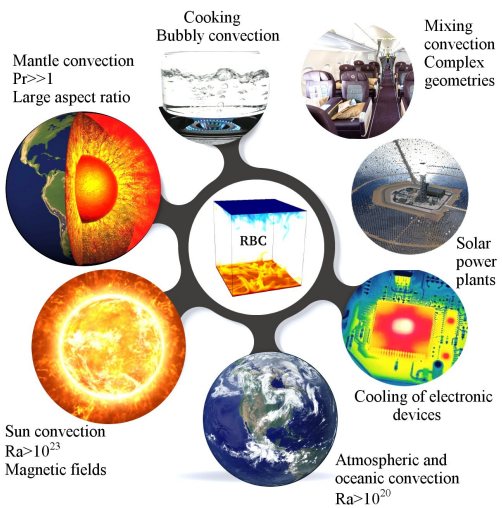
DNS

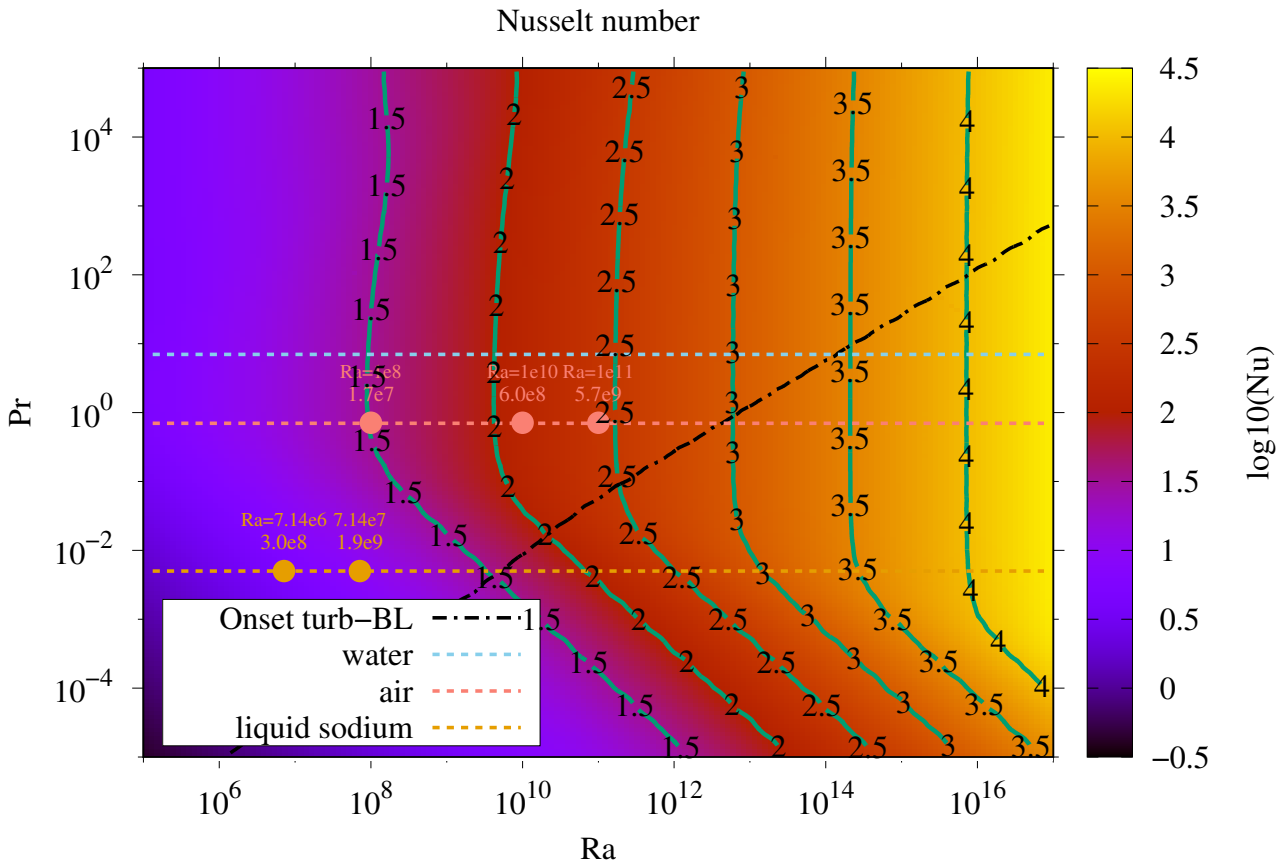
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LES of RBC

Research question #2:

- Can we hit the ultimate regime of thermal turbulence ?

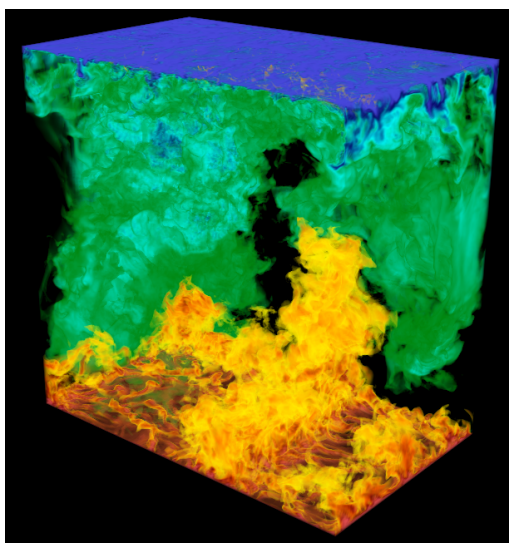


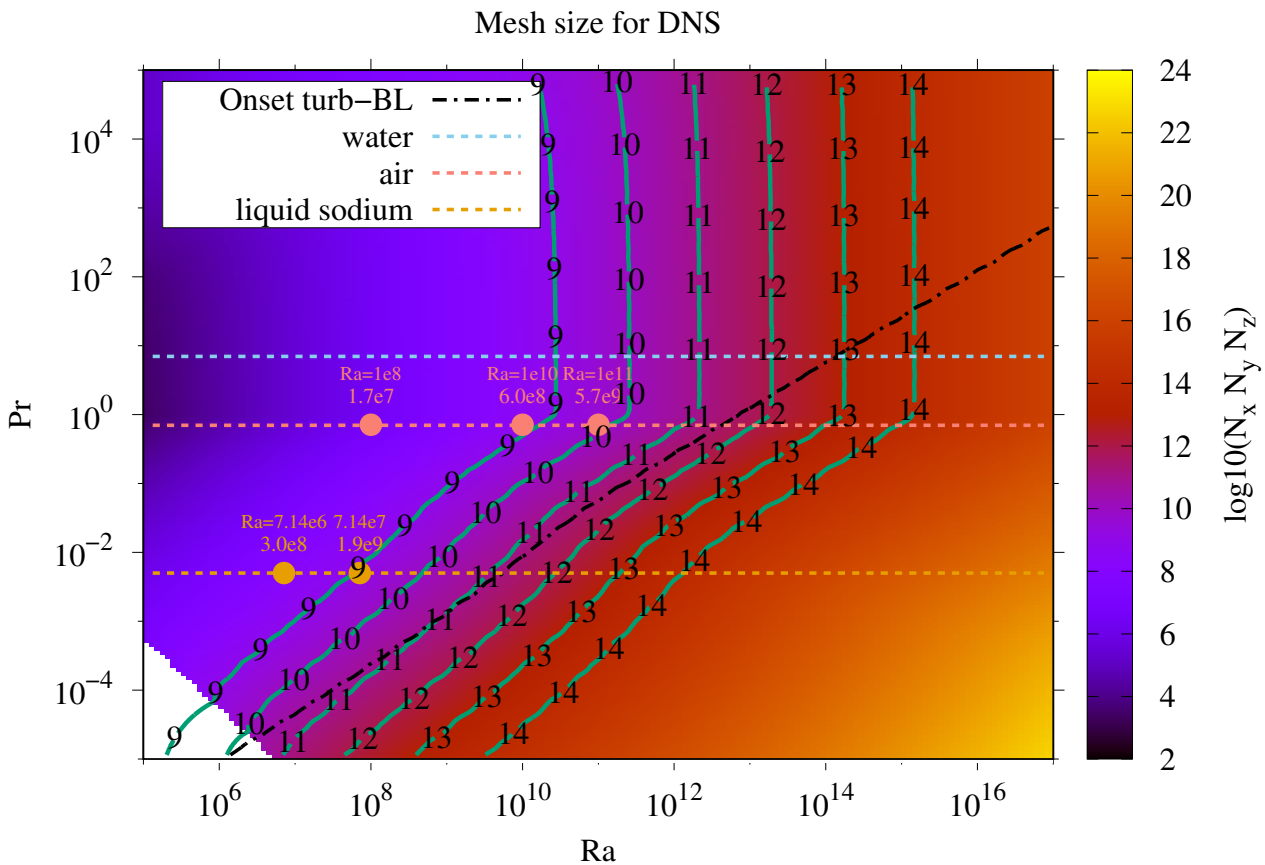


LES of RBC

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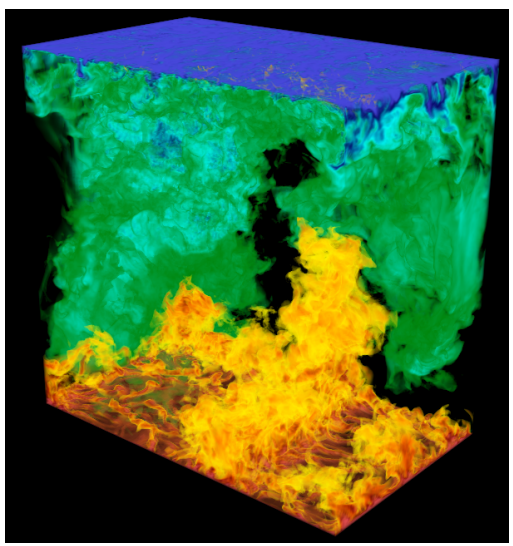


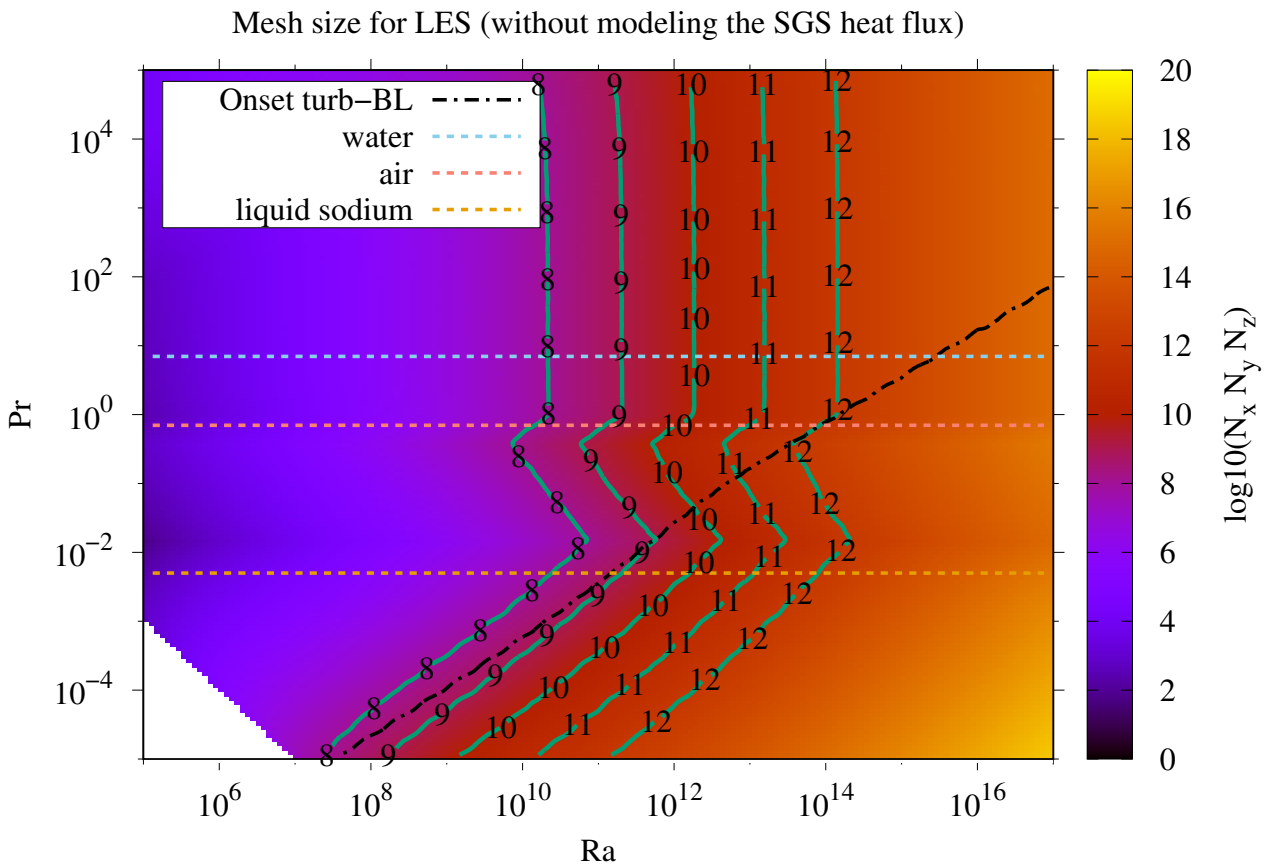


LES of RBC

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Problems to model the SGS heat flux[8]

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

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eddy-diffusivity

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

gradient model

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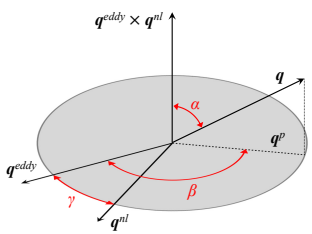
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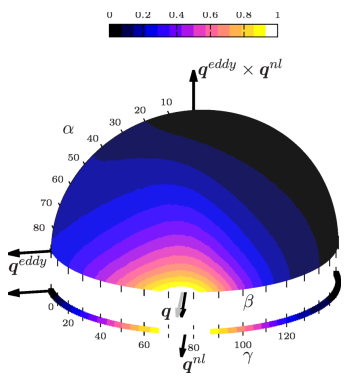
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eddy-viscosity $\longrightarrow \quad \tau\ (\overline{\boldsymbol{u}}) = -2\nu_t S(\overline{\boldsymbol{u}})$

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

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

eddy-diffusivity

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

gradient model

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

[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.

DNS results at very low Pr number

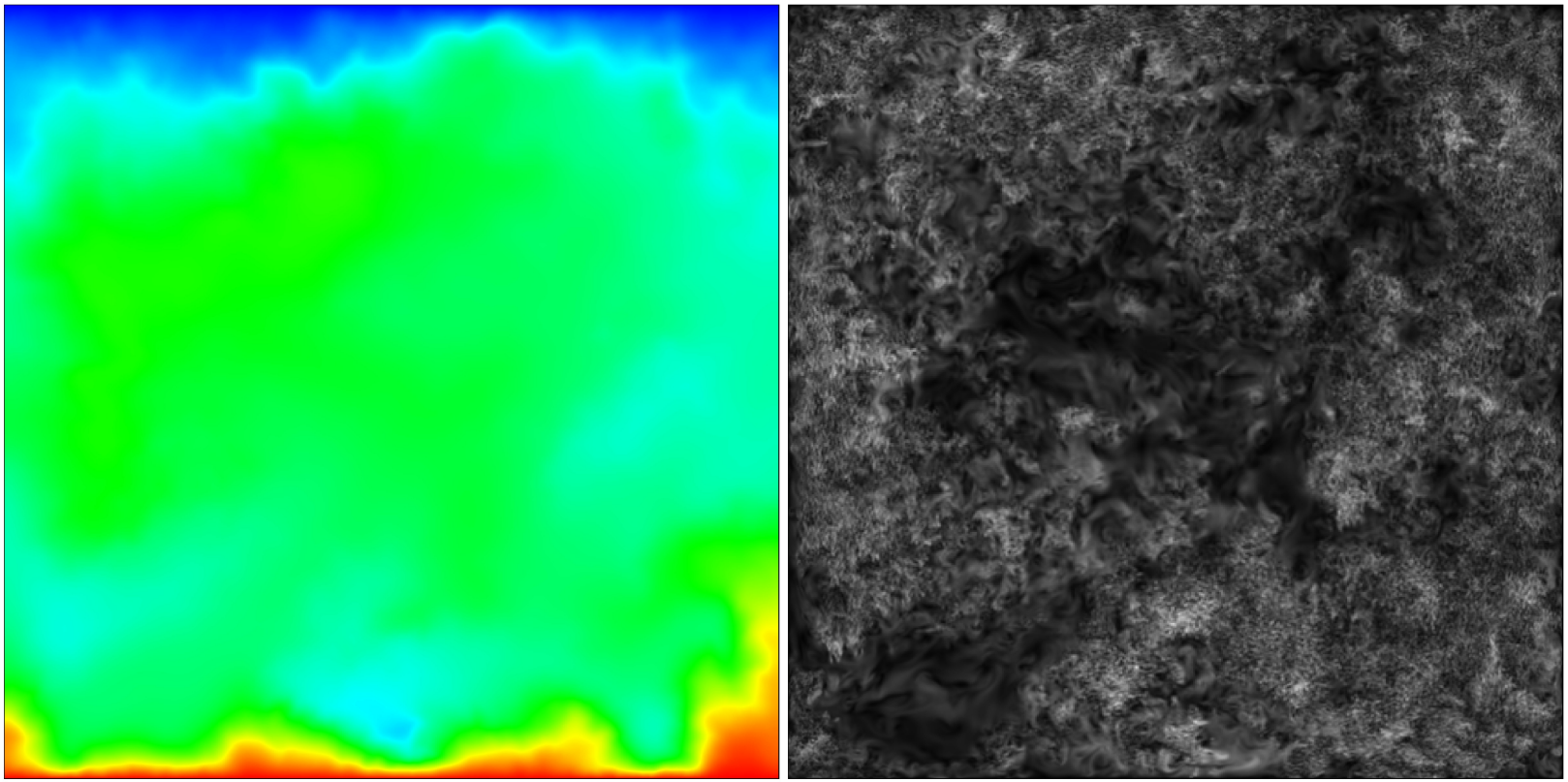
Why? scale separation grows as $\eta_K/\eta_T = Pr^{3/4}$.

η_T: Obukhov-Corrsin scale; η_K: Kolmogorov scale

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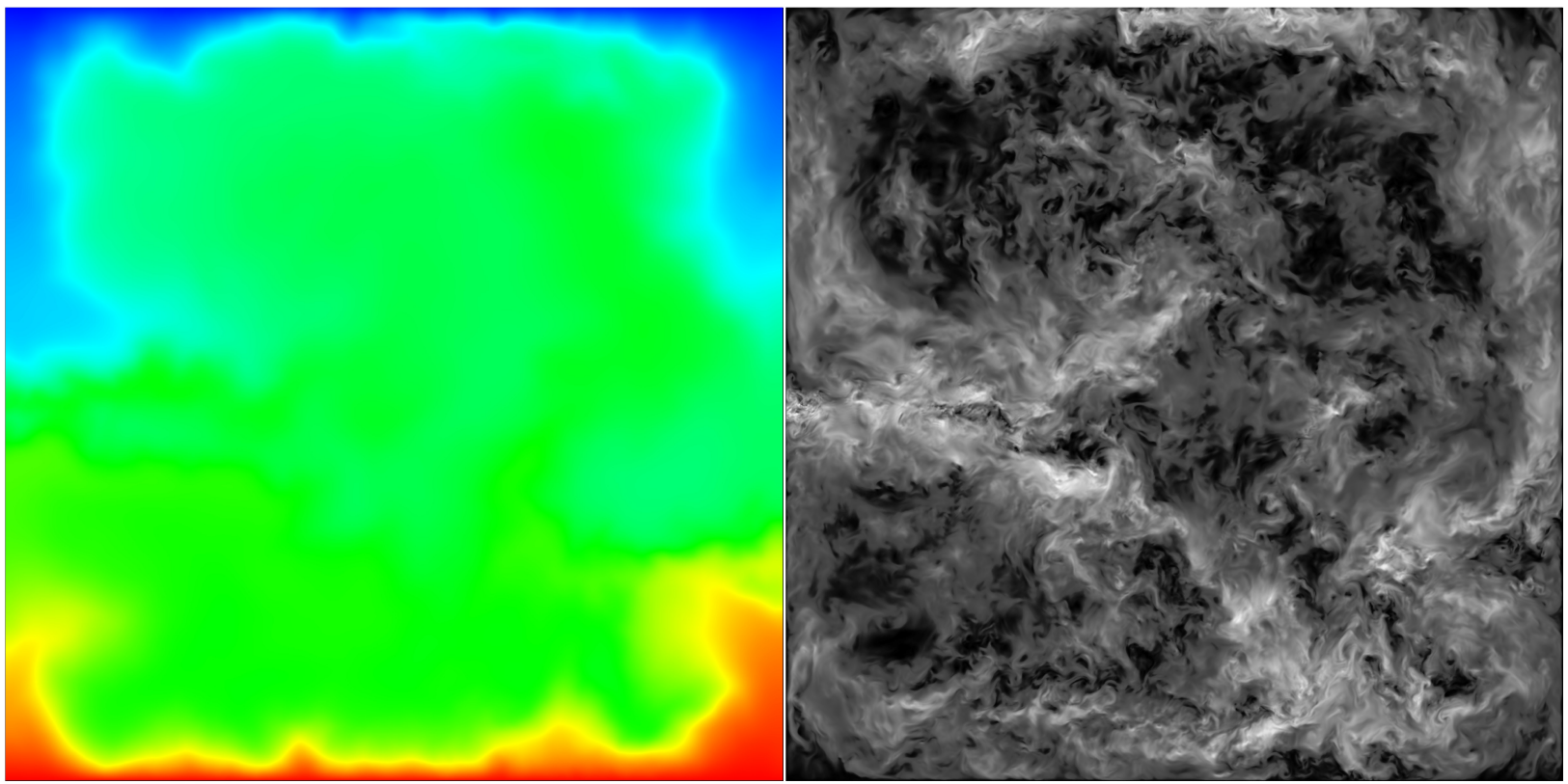
DNS of a RB at $Ra = 7.14 \times 10^6$ and $Pr = 0.005$ (liquid sodium)

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

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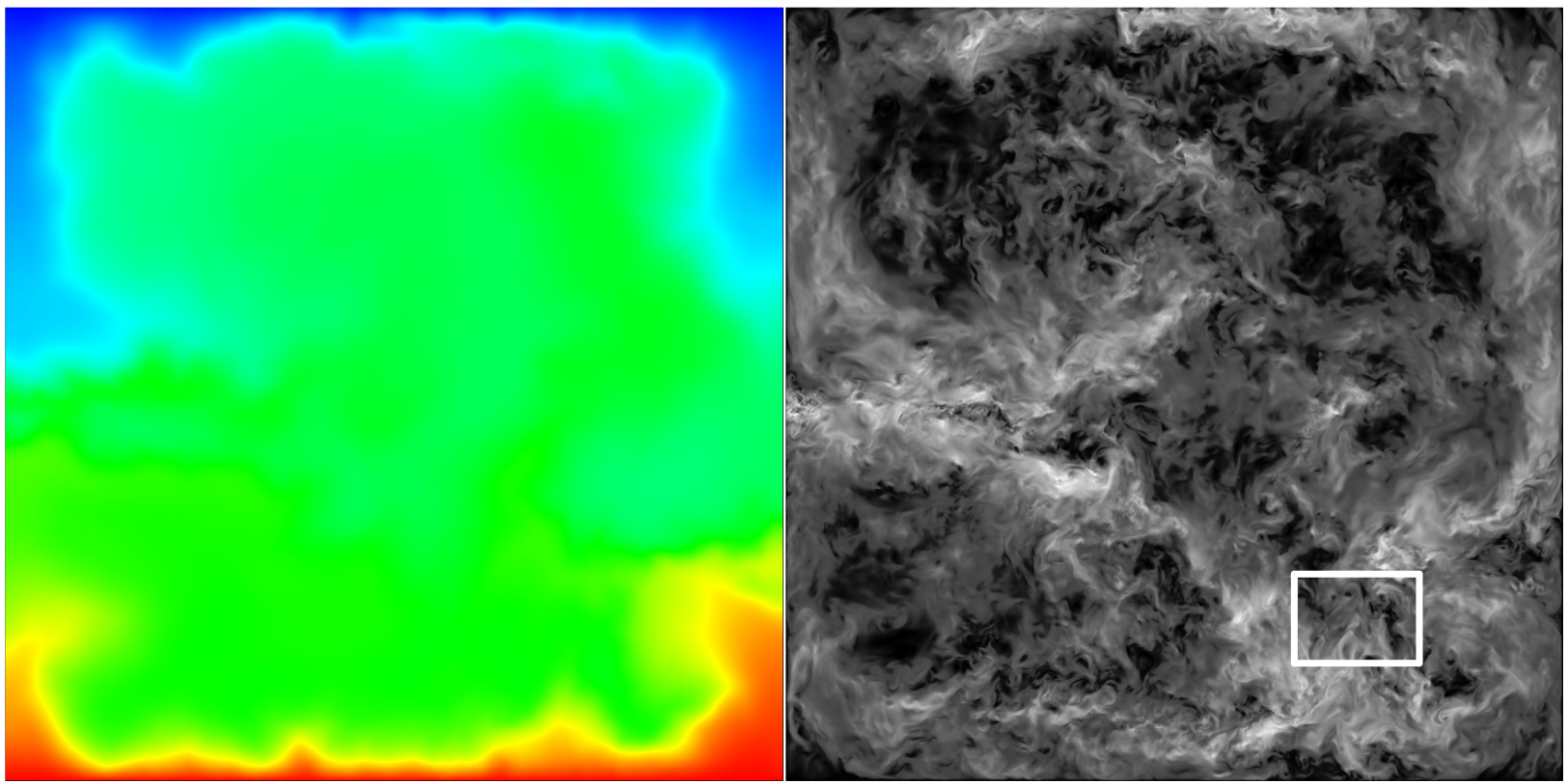
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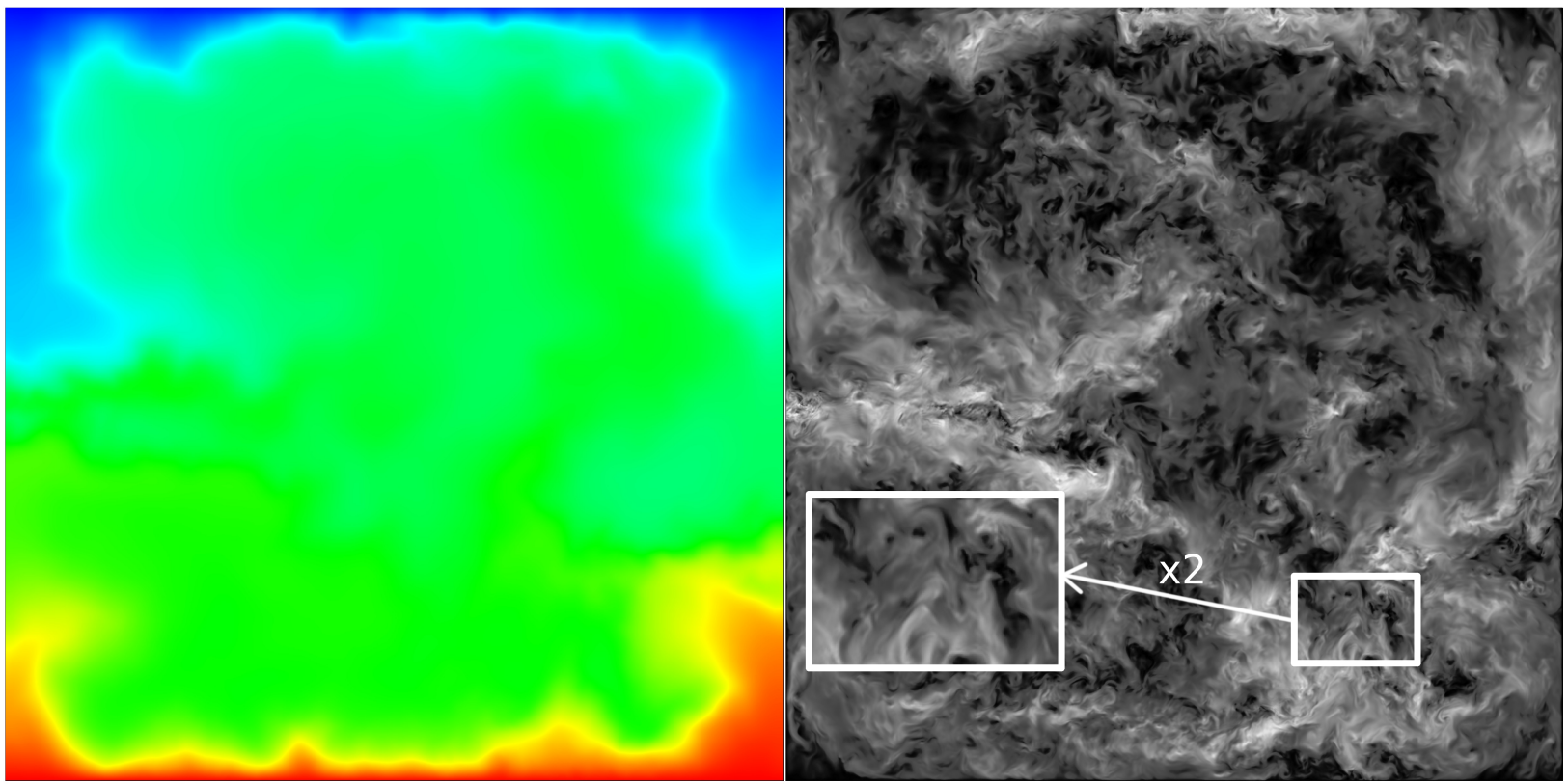
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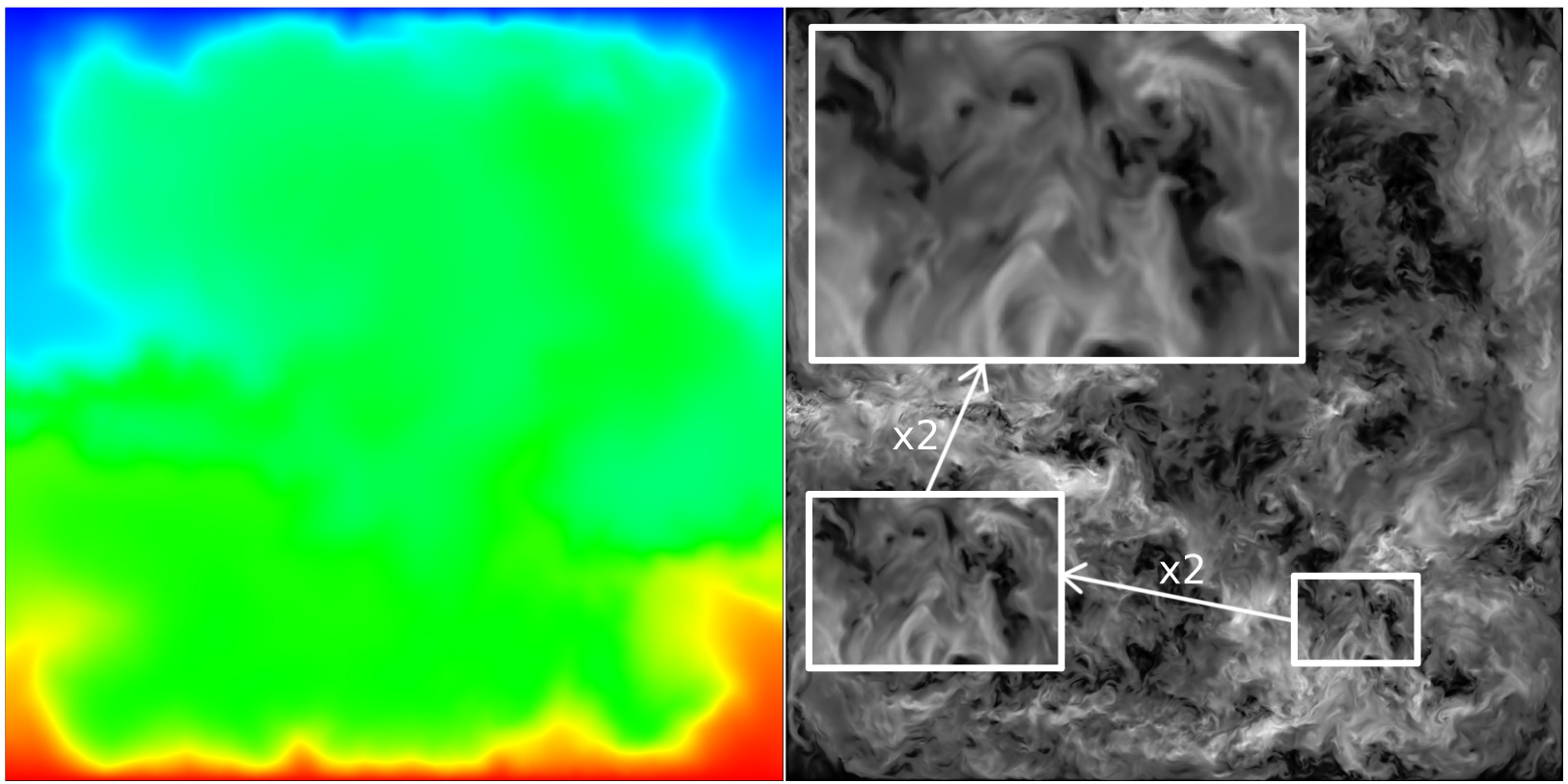
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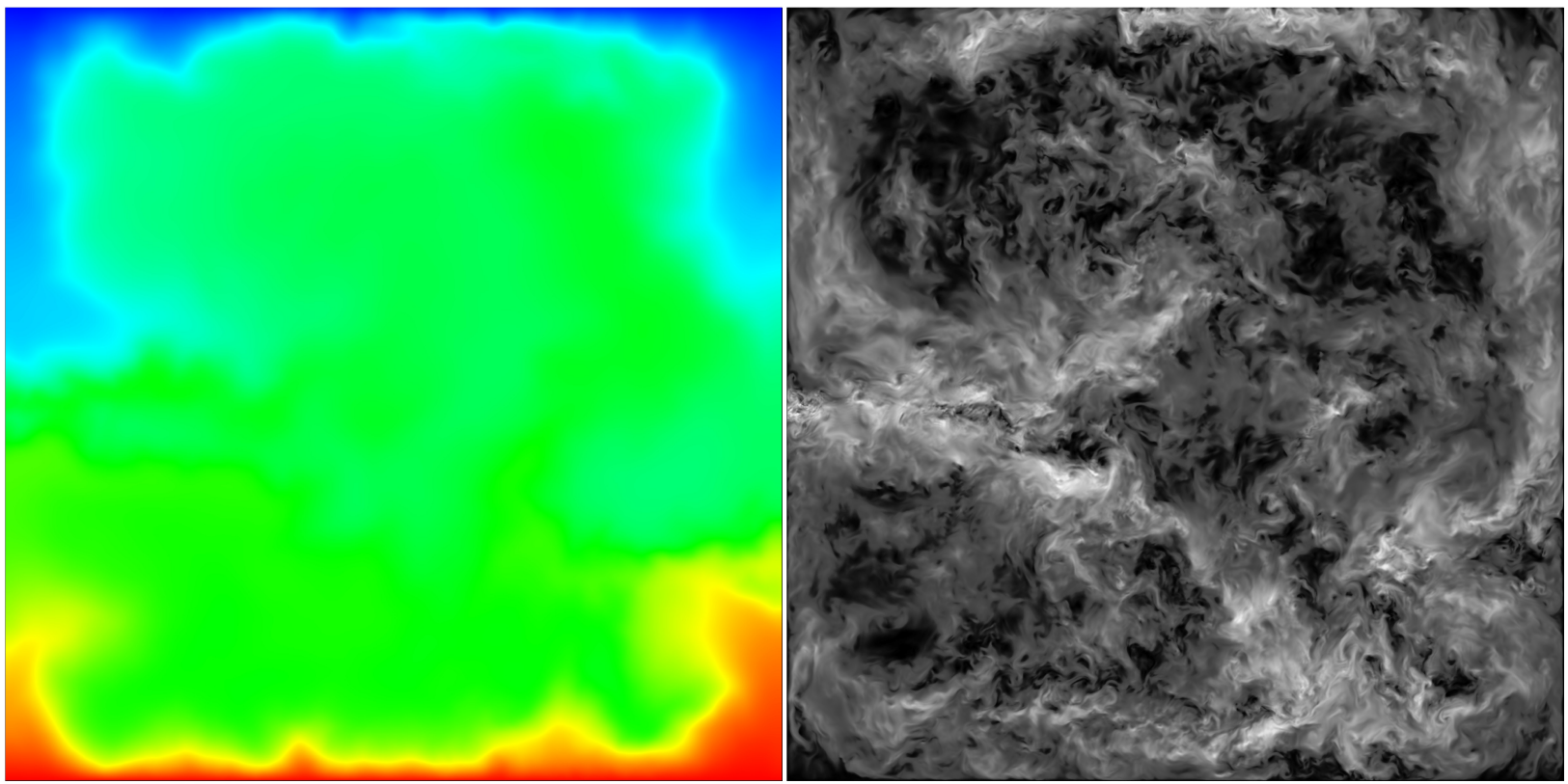
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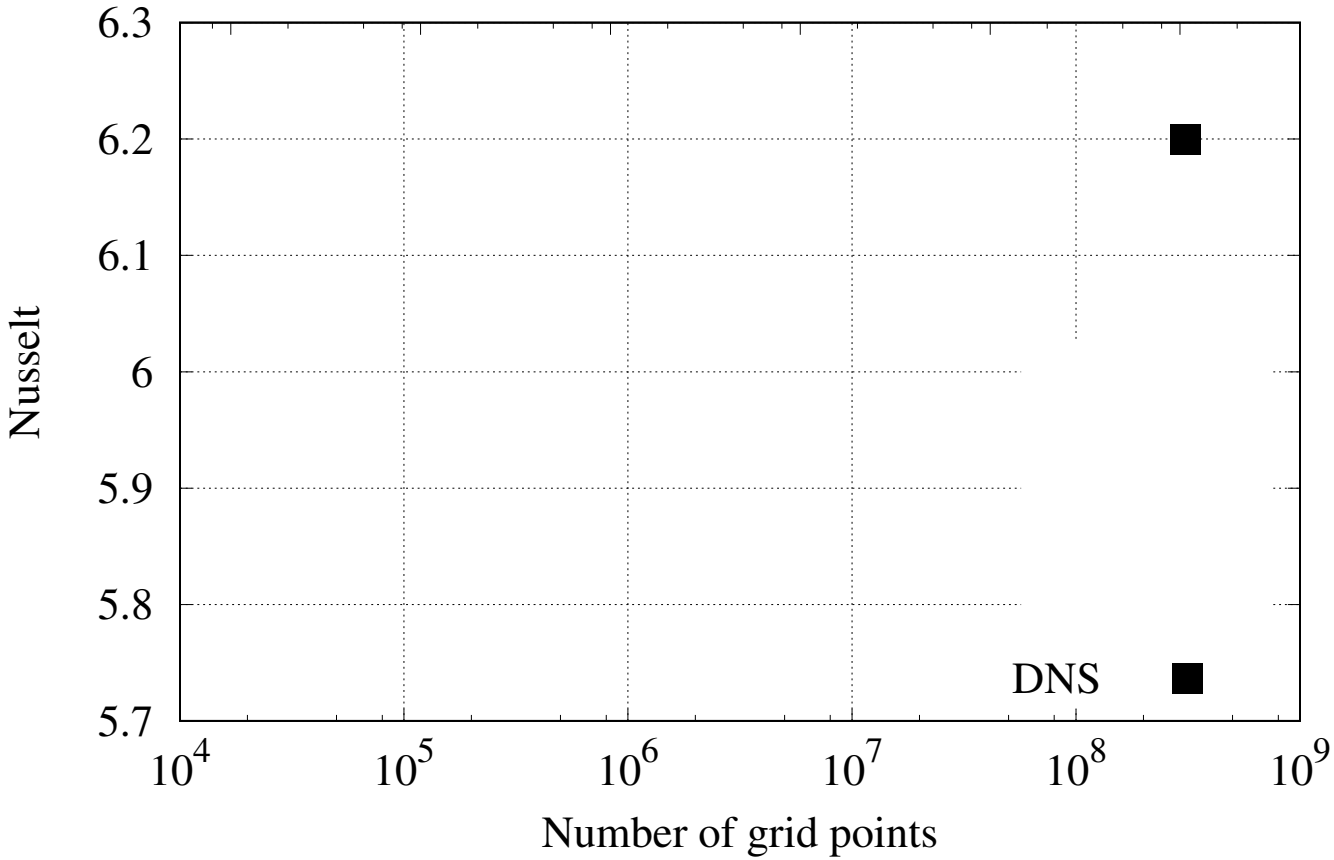


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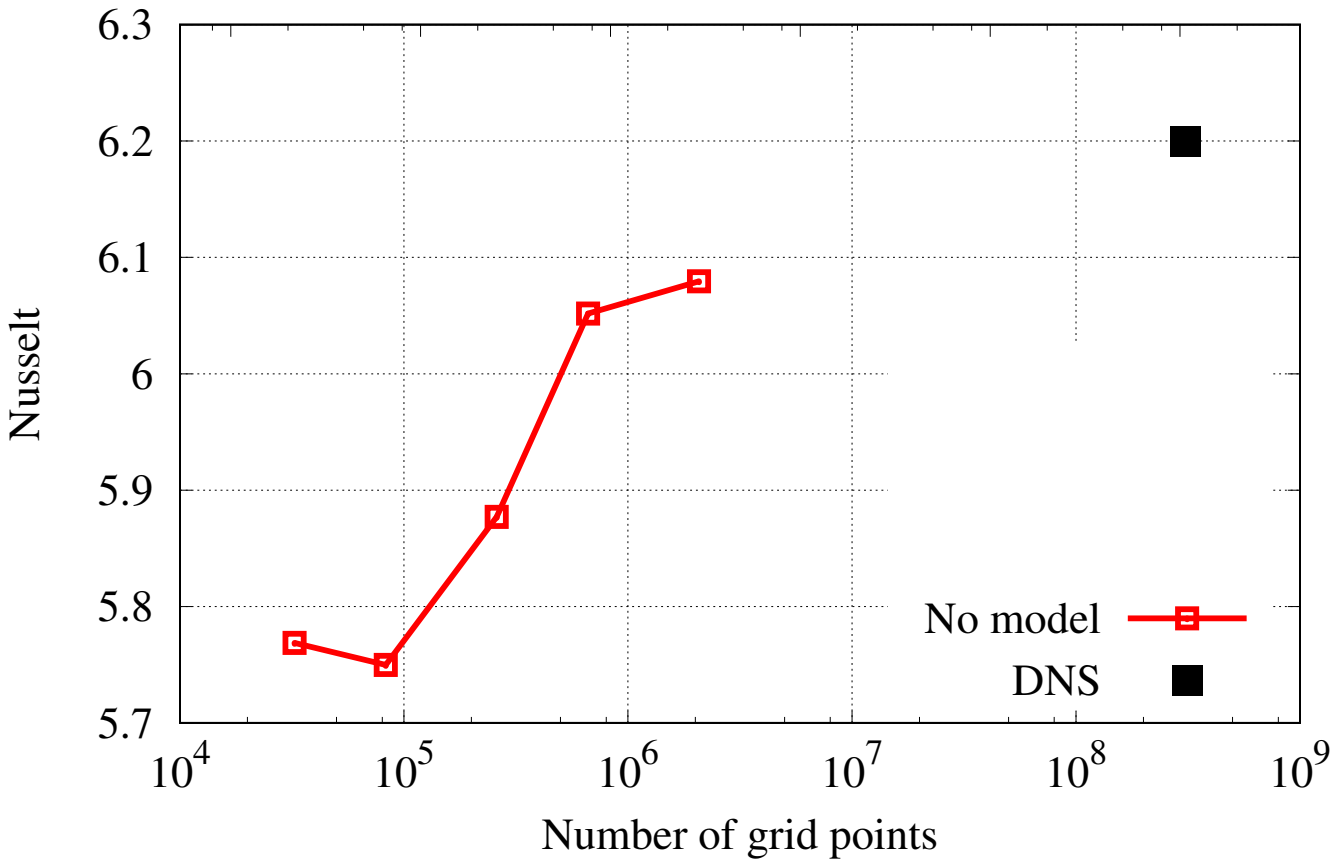
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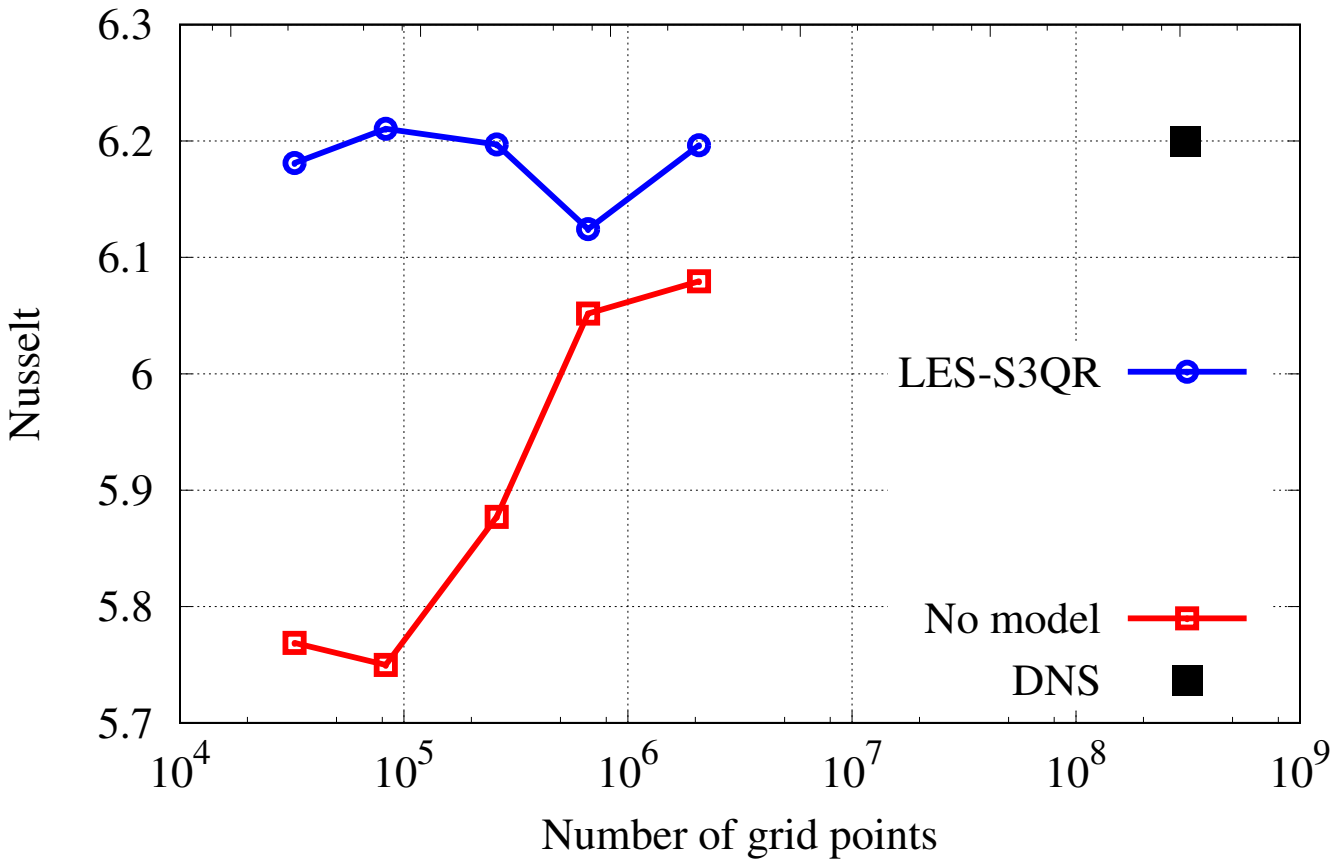
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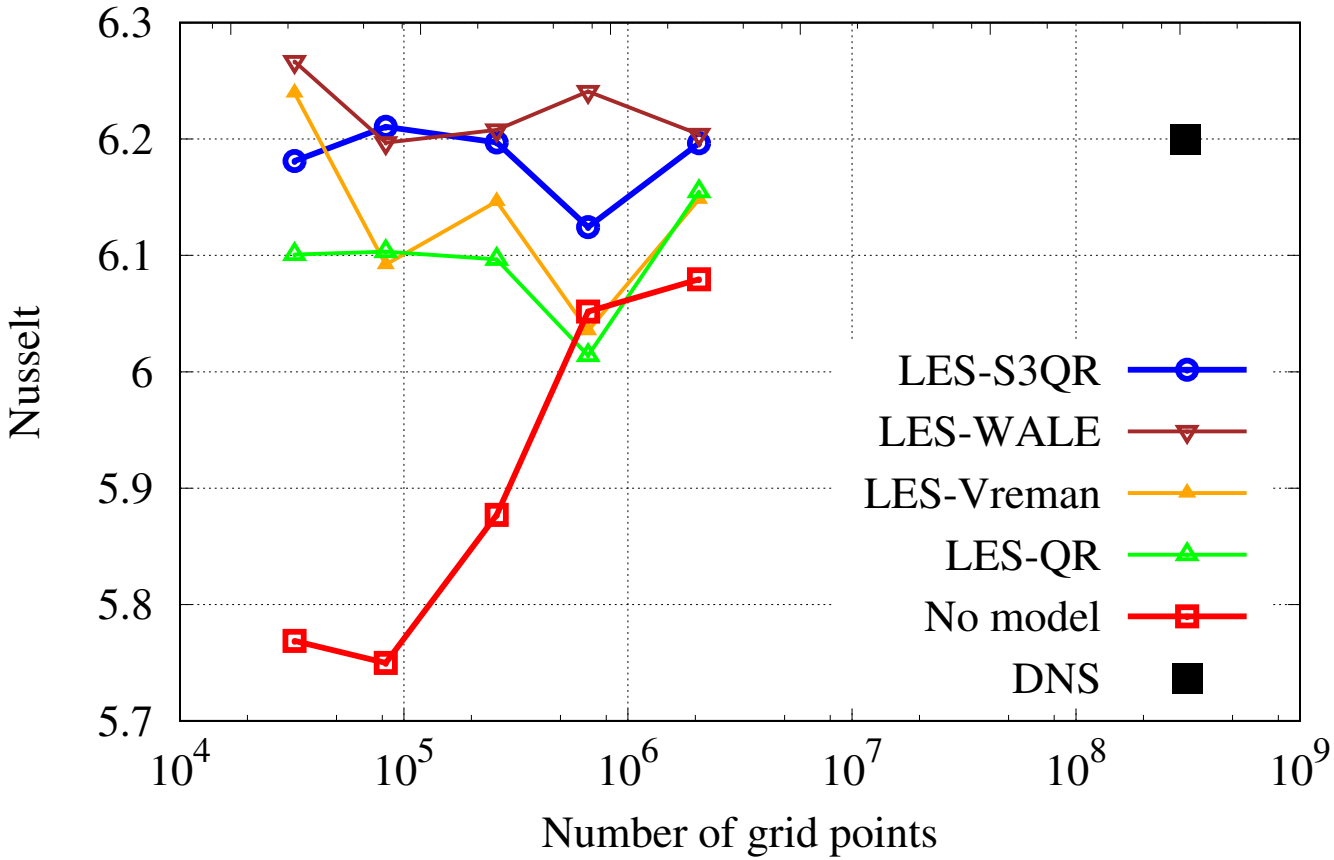
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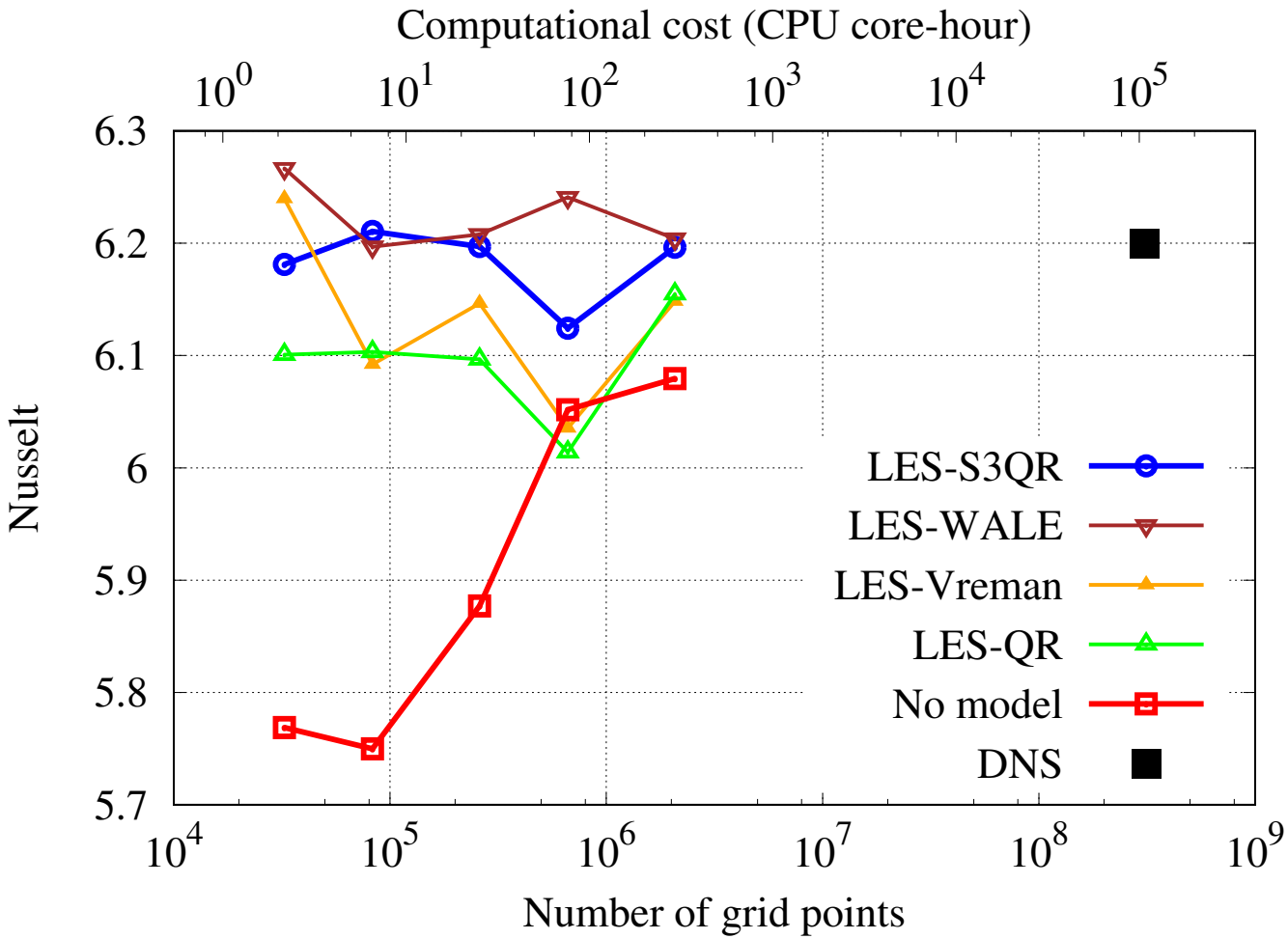
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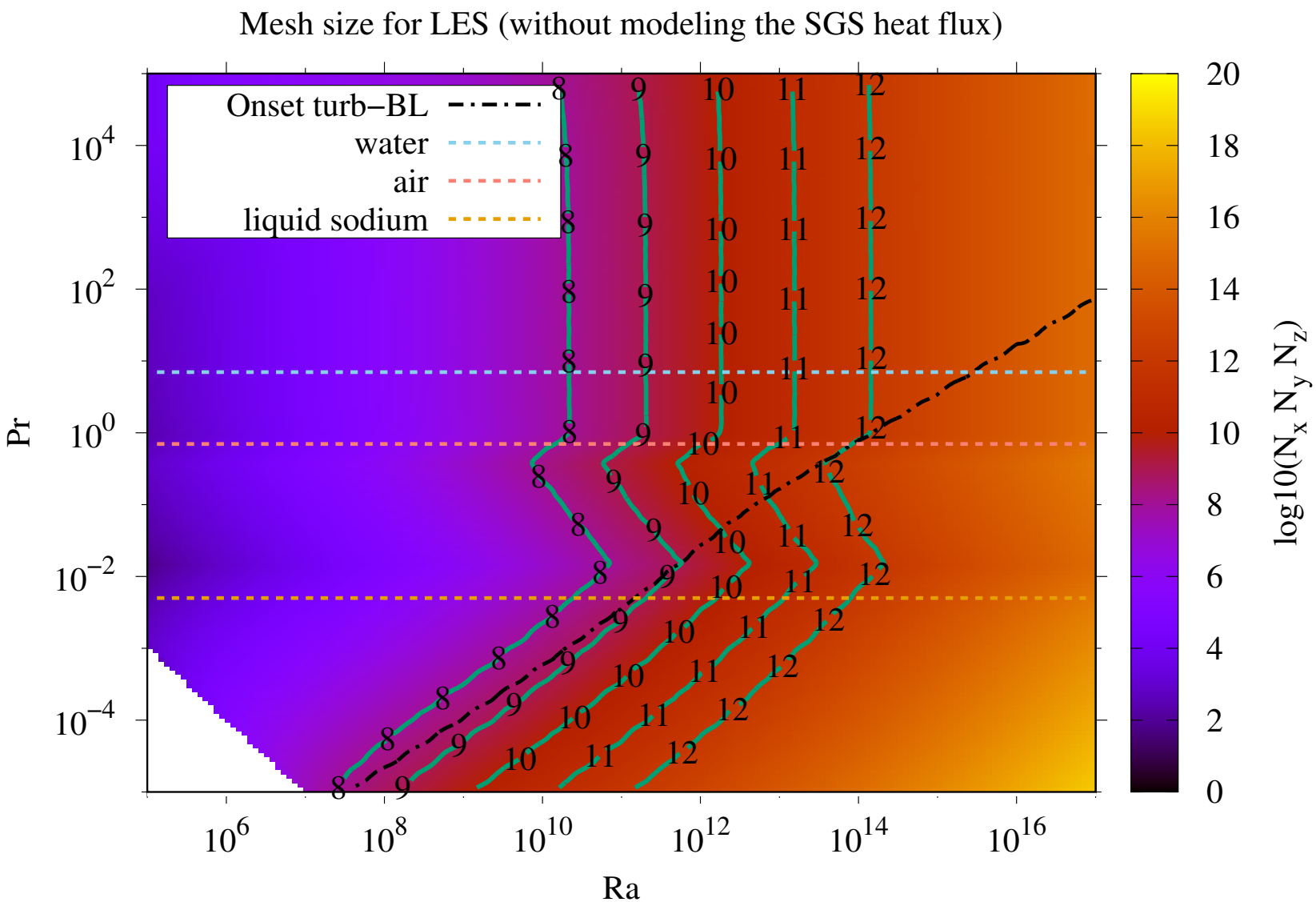
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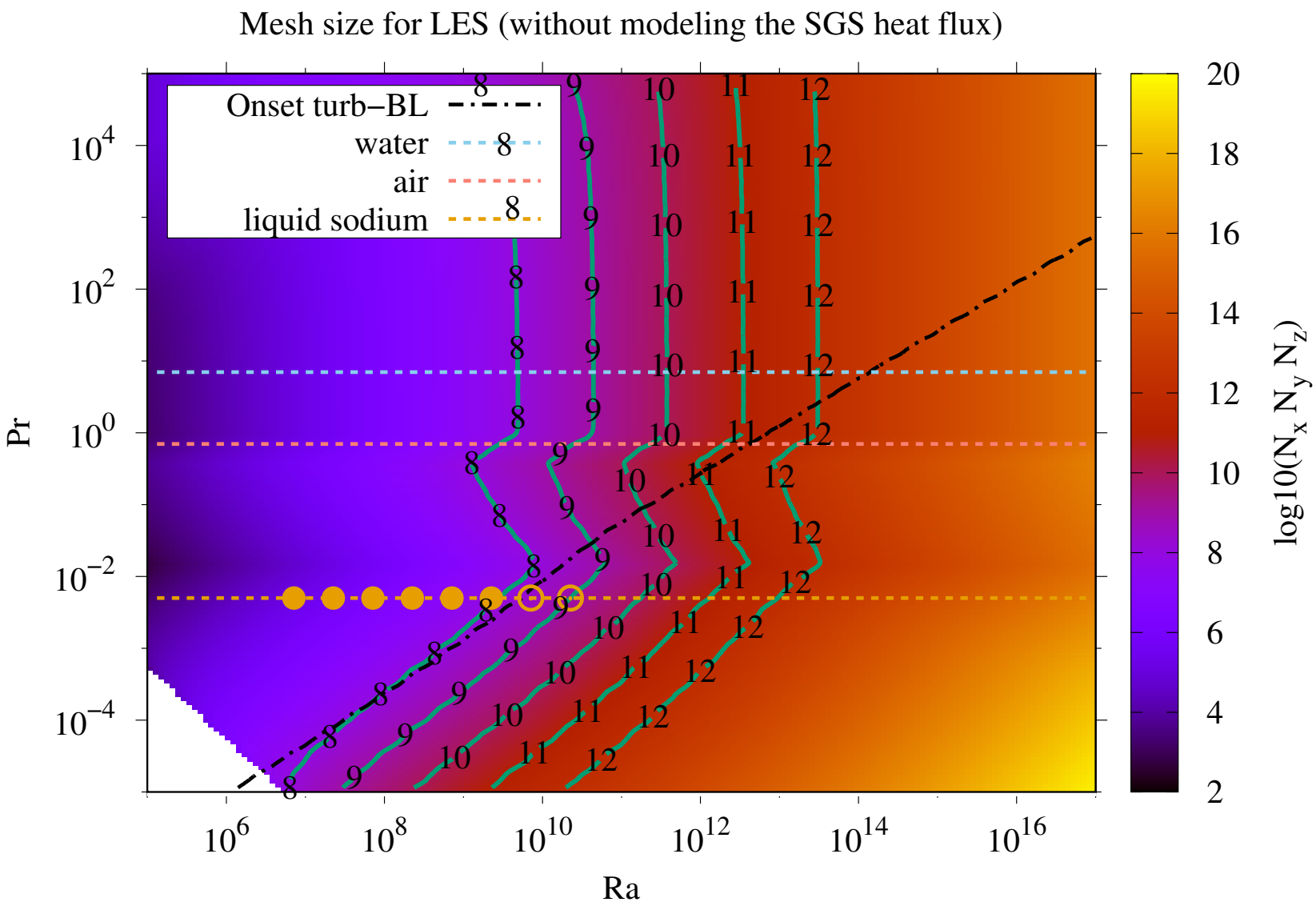


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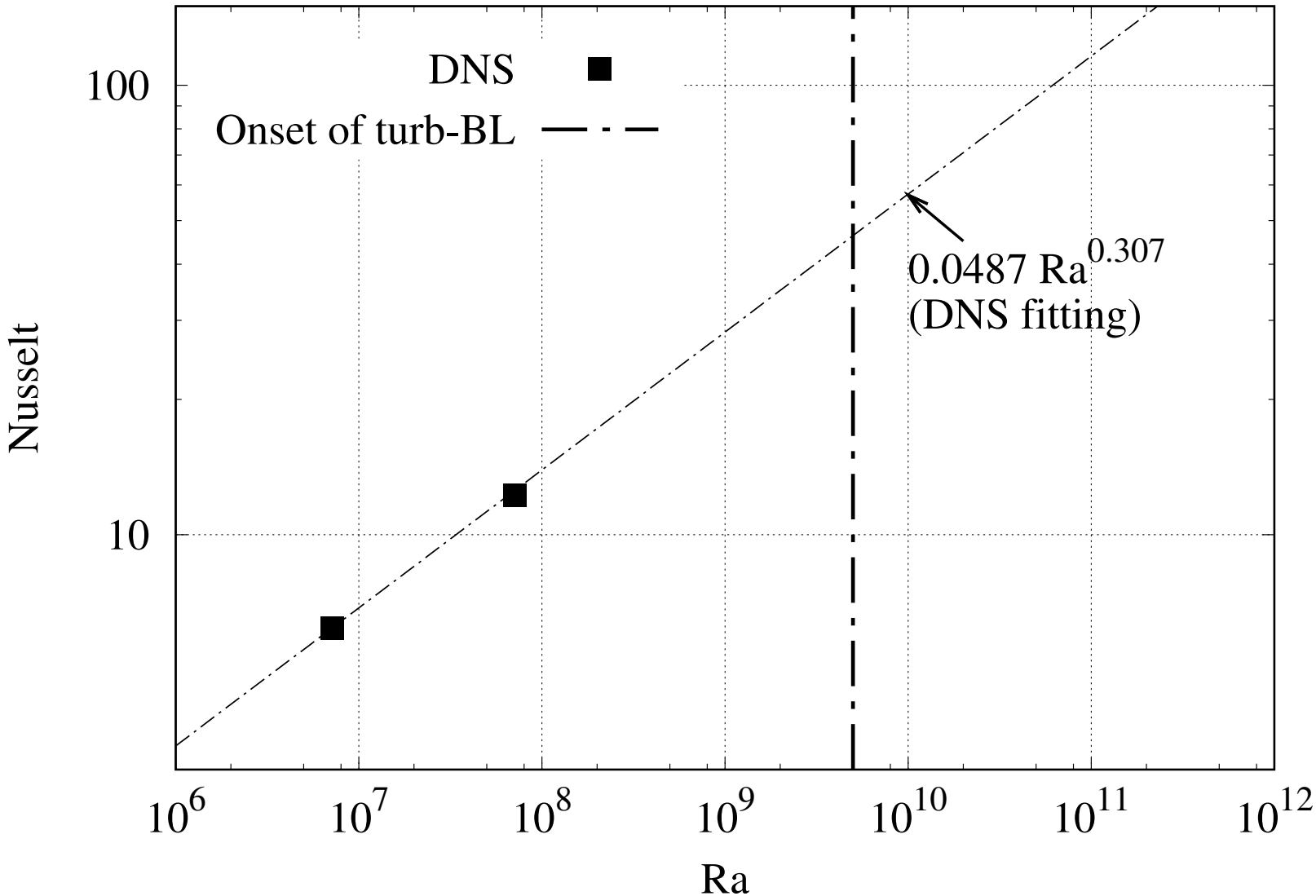
LES results at very low *Pr* number



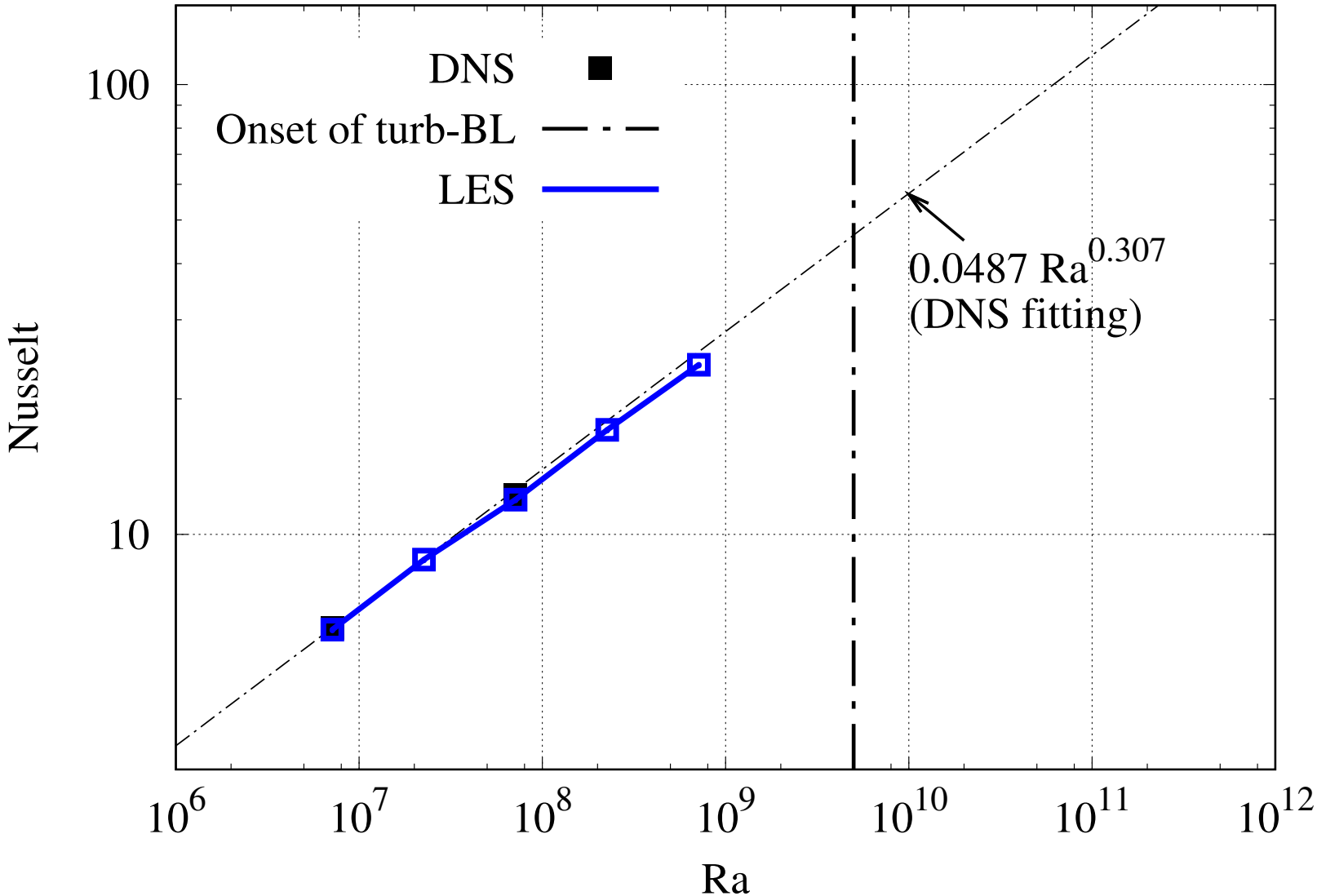
LES results at very low *Pr* number (on-going)



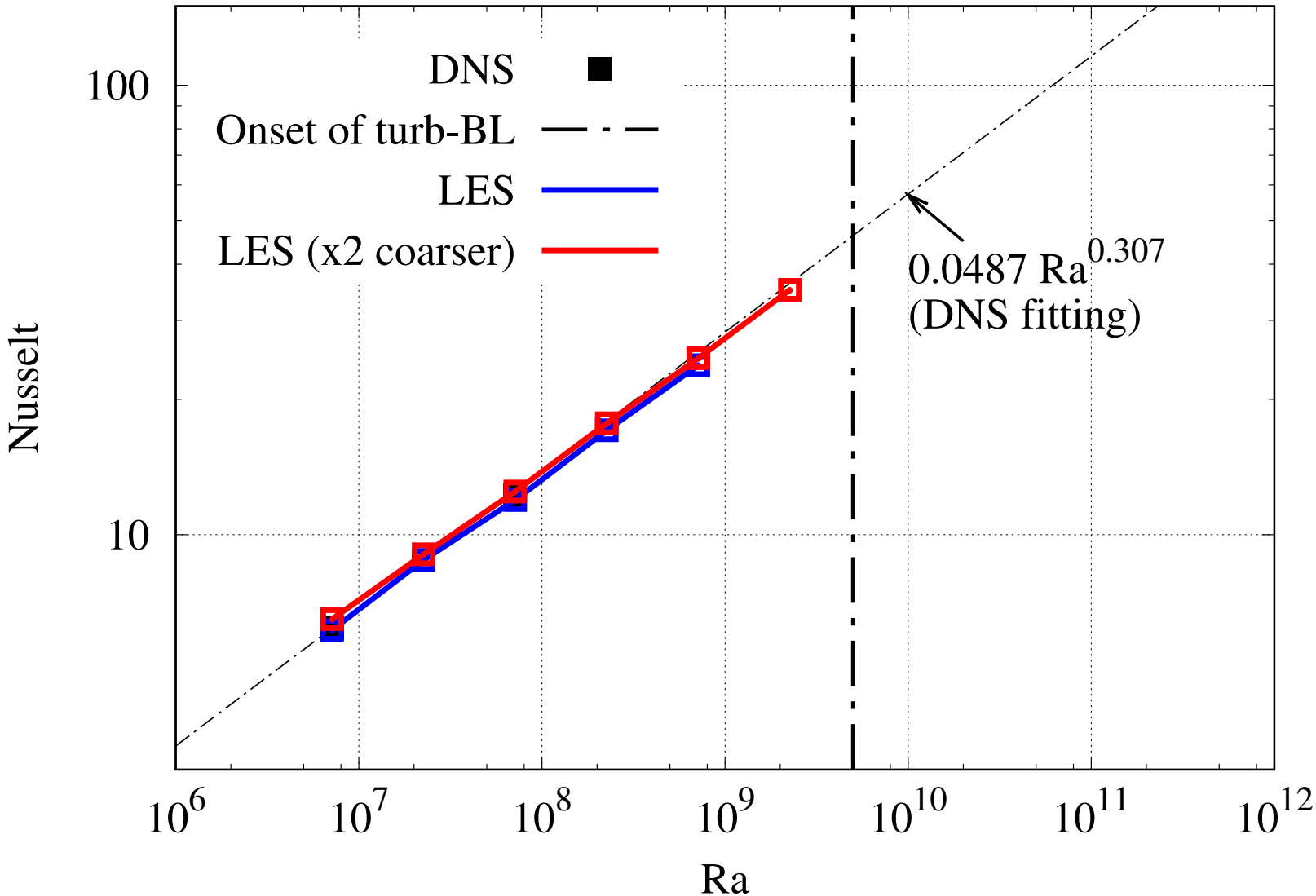
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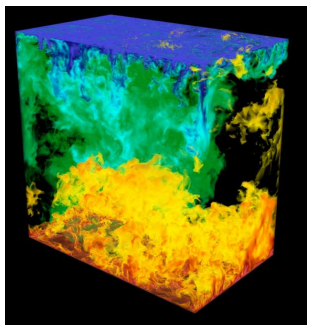
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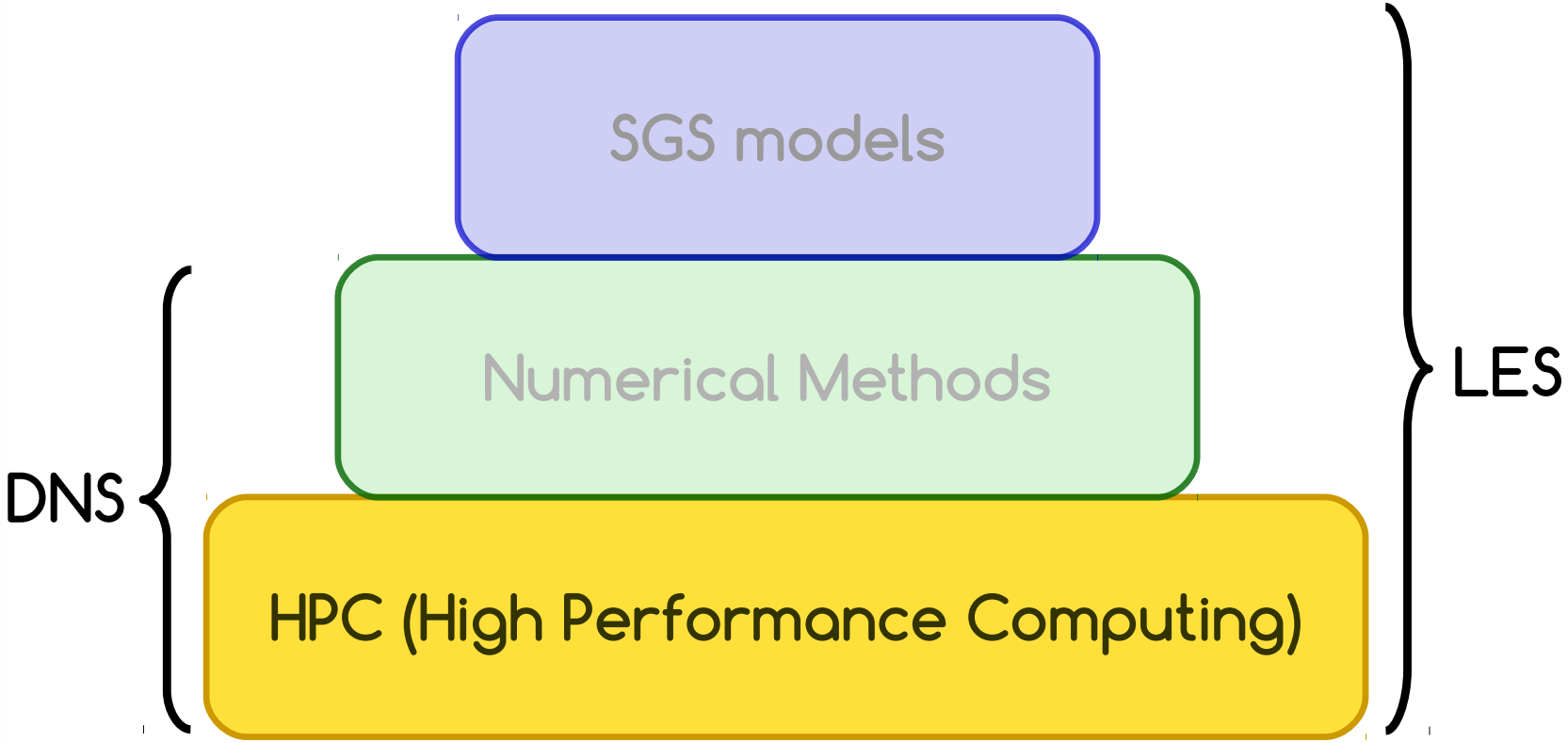


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HPC on modern supercomputers

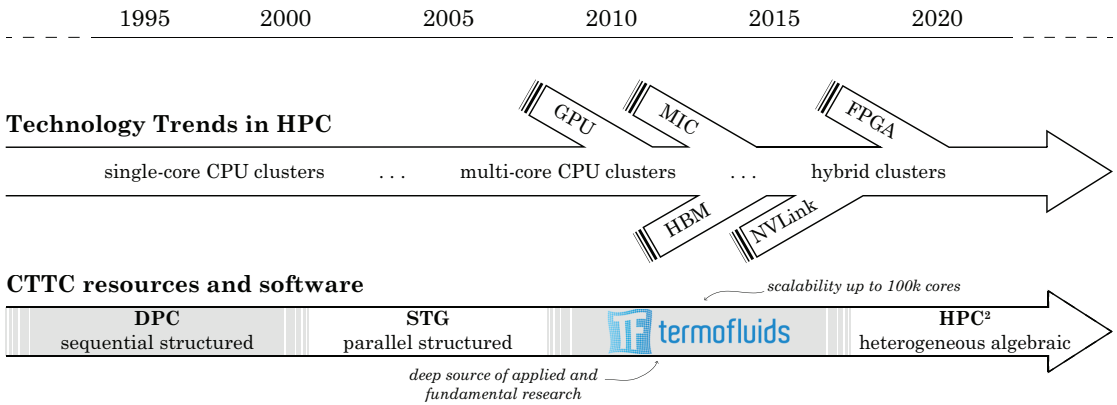




HPC on modern supercomputers

Research question #3:

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



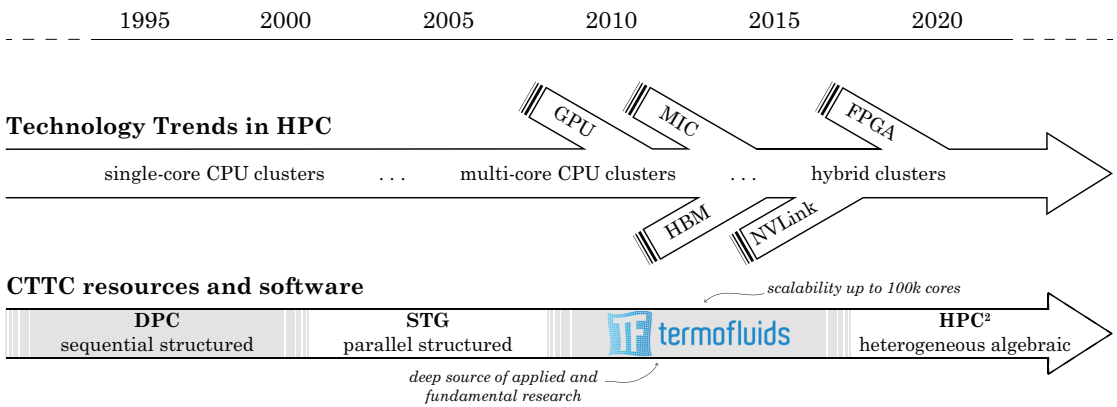
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HPC²: portable, algebra-based framework for heterogeneous computing is being developed[10]. Traditional stencil-based data and sweeps are replaced by algebraic structures (sparse matrices and vectors) and kernels. SpMM-based strategies to increase the arithmetic intensity are under development[11].

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Algebra-based approach naturally leads to portability, to simple and analyzable formulations

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

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Discrete

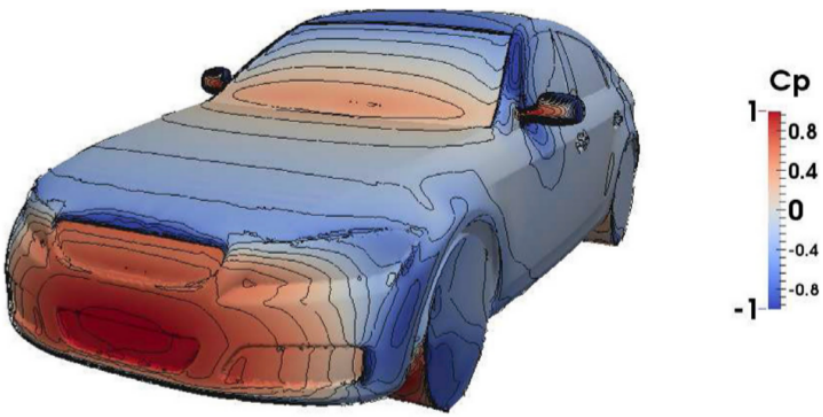
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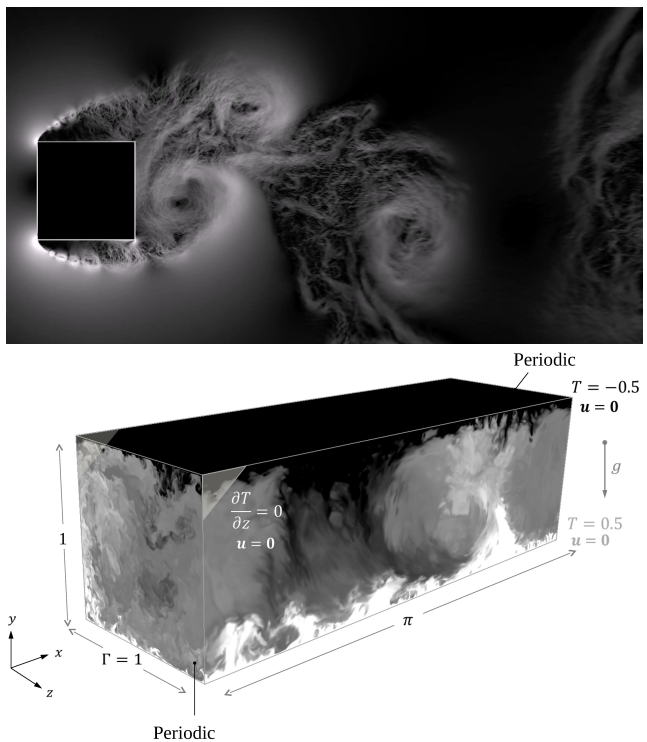
$$M\boldsymbol{u}_h = \boldsymbol{0}_h$$

Minimal set of kernels:

$$\texttt{SpMM}: \quad \boldsymbol{y} \leftarrow A\boldsymbol{x}$$
$$\texttt{axpy}: \quad \boldsymbol{z} \leftarrow a\boldsymbol{x} + b\boldsymbol{y}$$
$$\texttt{dot}: \quad r \leftarrow \boldsymbol{x} \cdot \boldsymbol{y}$$

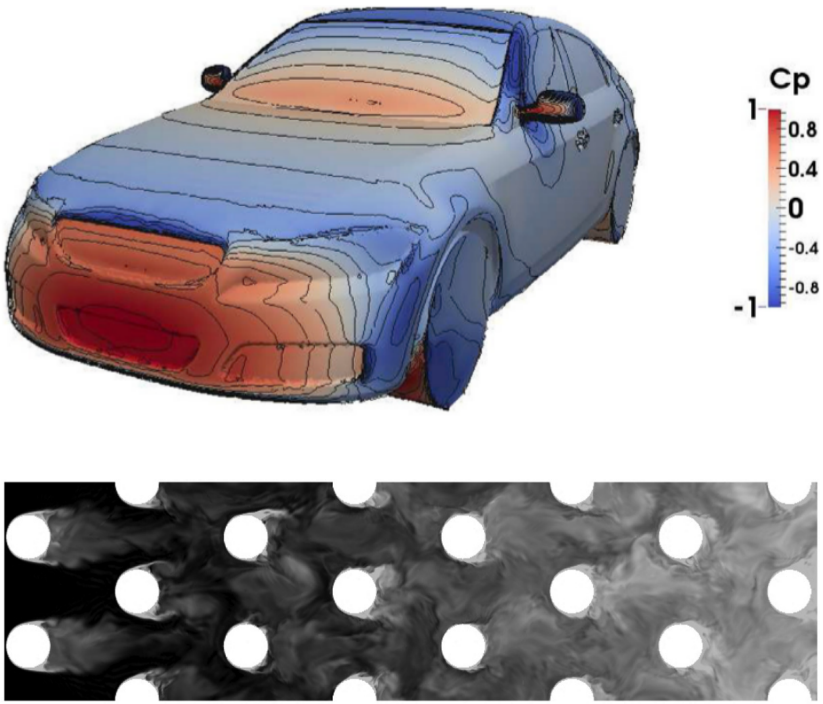
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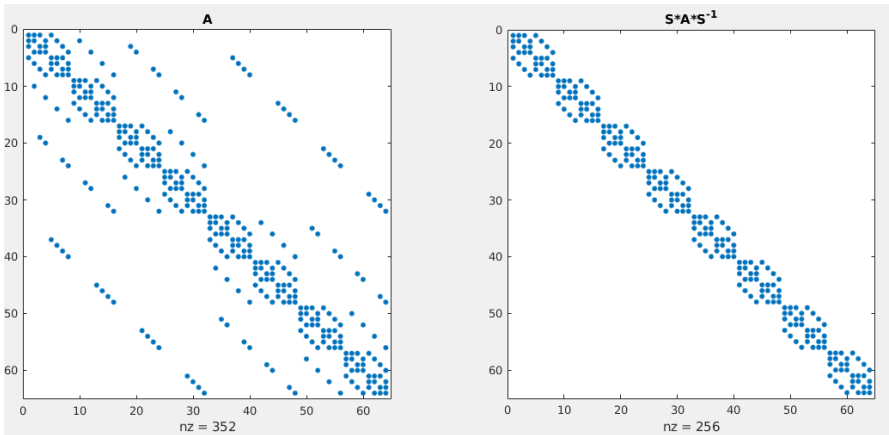


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SpMM can be used $\Longrightarrow$ **higher AI**

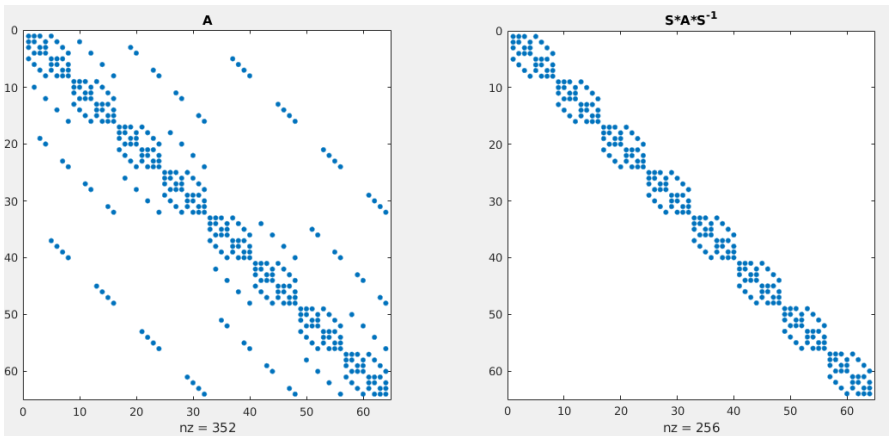
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Benefits for Poisson solver are 3-fold:

- Higher arithmetic intensity (AI)
- Reduction of memory footprint
- Reduction in the number of iterations

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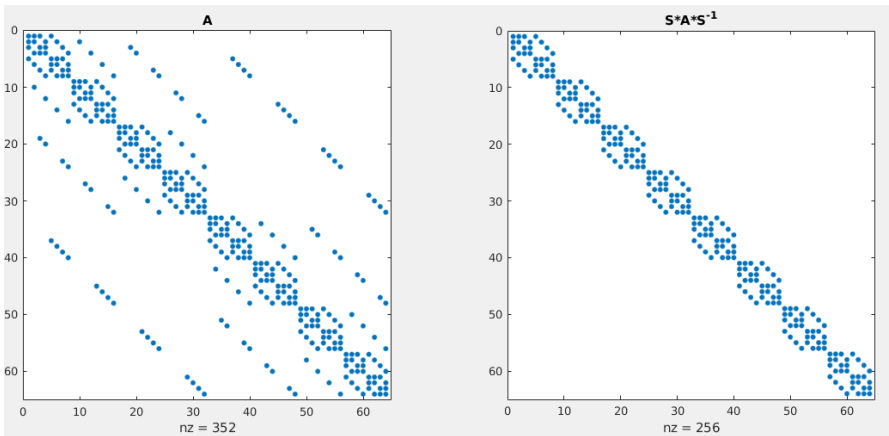
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→ Overall speed-up up to **x2-x3** ✓
→ Memory reduction of ≈**2** ✓

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SpMM can be used ⟹ **higher AI**

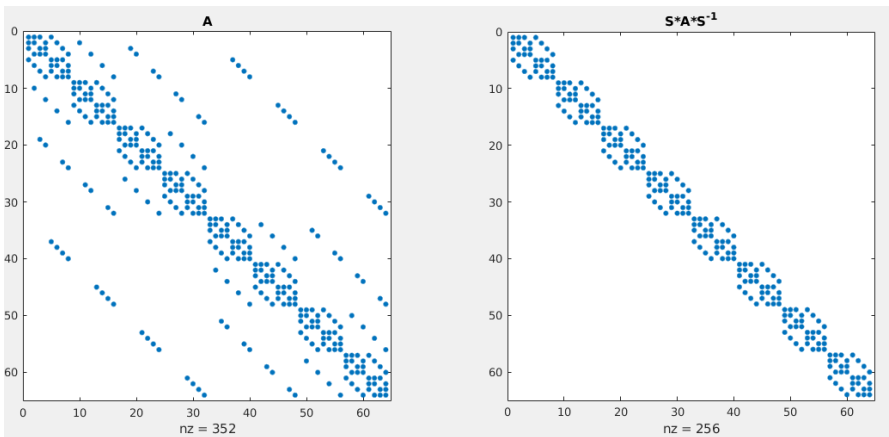
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Other SpMM-based strategies to **increase AI** and **reduce memory** footprint:

- Multiple transport equations
- Parametric studies
- Parallel-in-time simulations
- Go to higher-order?

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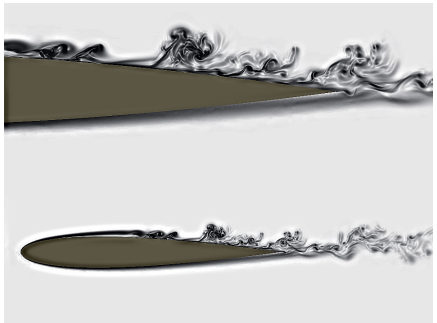


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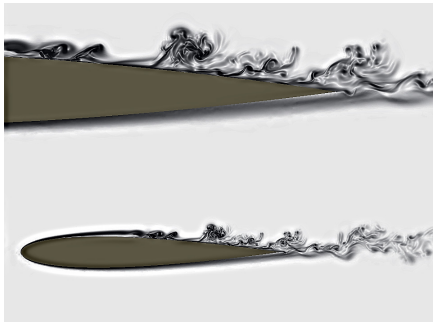
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Concluding remarks

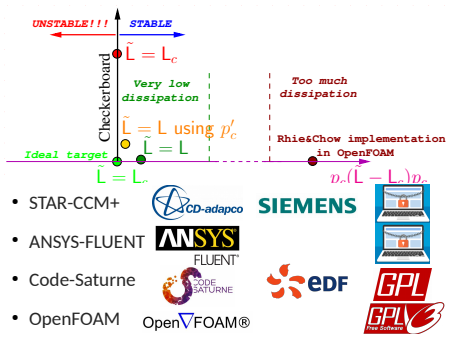
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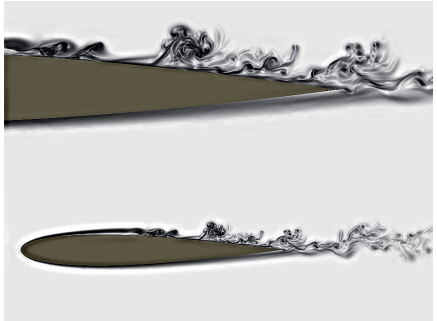
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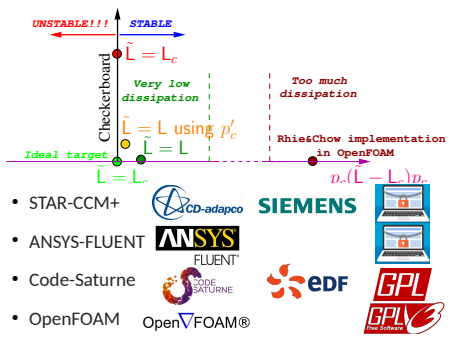
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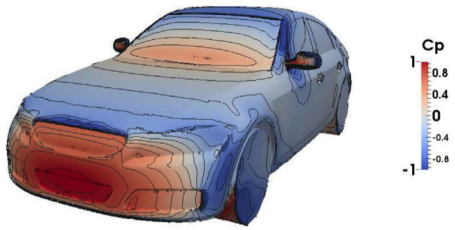


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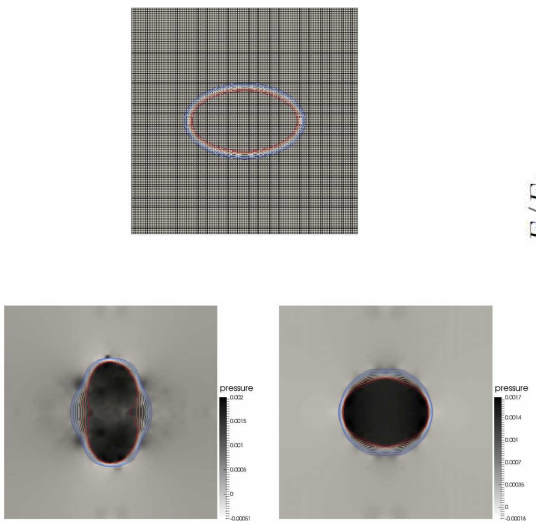
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- Main drawback of **collocated** formulations: you either have **checkerboard** or some (small) amount of **artificial dissipation** due to pressure term.
- Algebra-based approach naturally leads to **portability**, to simple and **analyzable** formulations and opens the door to **new strategies to improve its perfomance**.

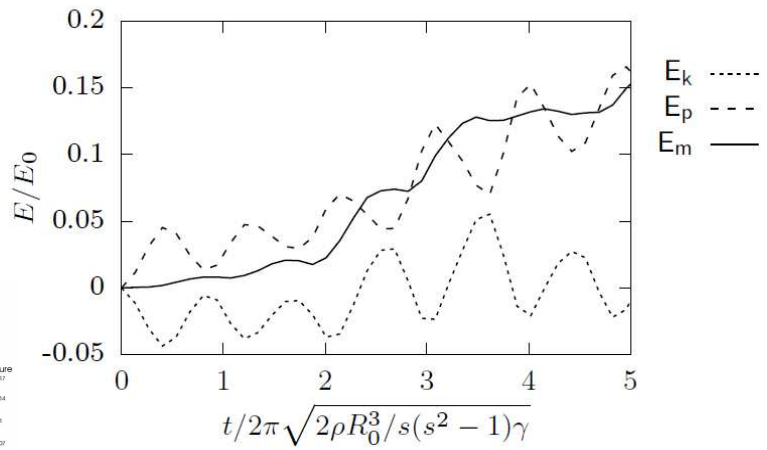




On-going (related) research

- **Rethinking** standard CFD operations (*e.g.* flux limiters[13], CFL[14],...) to adapt them into an algebraic framework (*Leitmotiv*: maintaining a minimal number of basic kernels is crucial for portability!!!)
- Symmetry-preserving formulations for **multiphase flows**[15]





Mechanical energy (kinetic+potential) is not preserved!

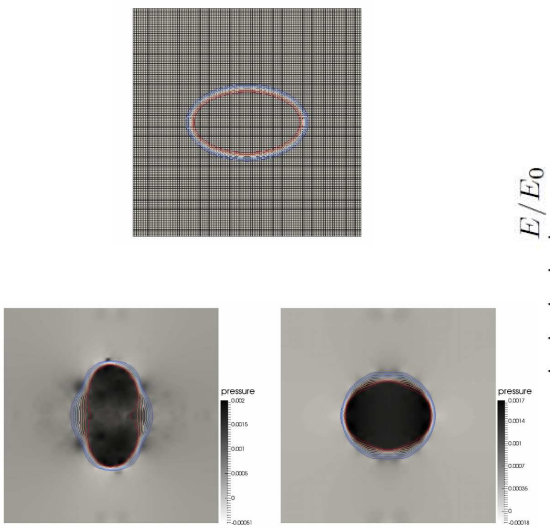
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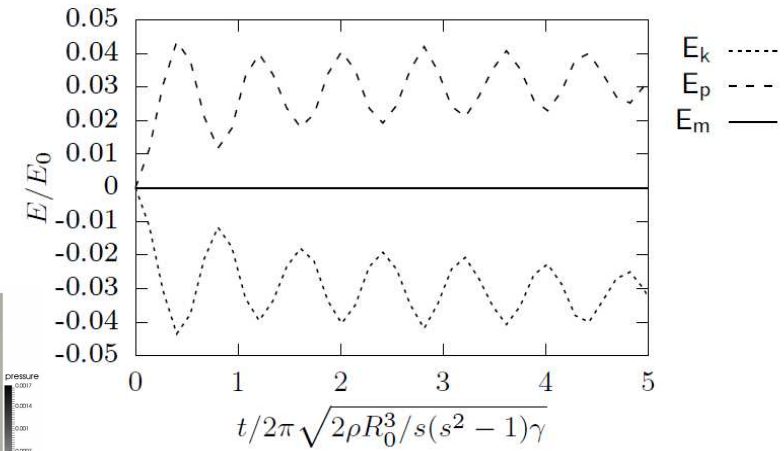
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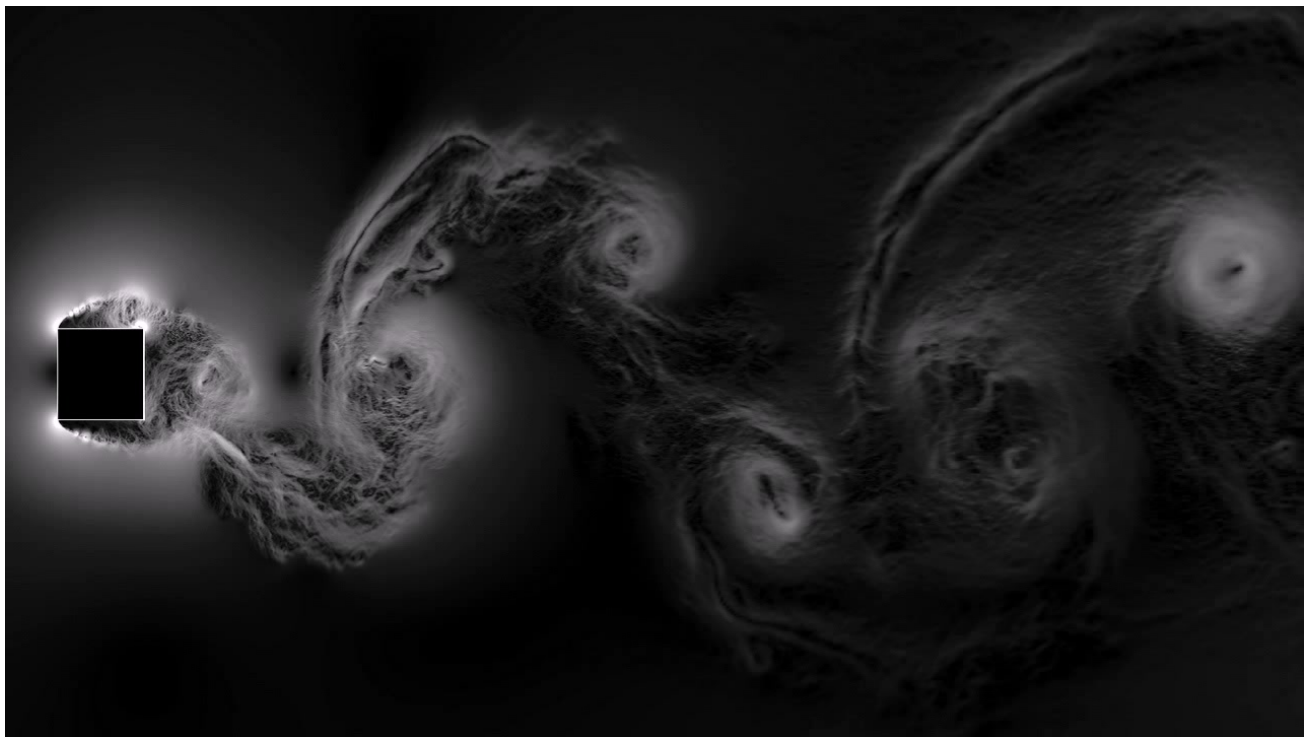
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Thank you for your attendance



Open questions and ideas for roundtable discussion

I. **Discrete conservation and turbulence modeling**
   Reconciling numerics with subgrid-scale modeling, ILES, LES, DES, ...

II. **Are we satisfied with the existing SGS models for LES?**
   Do we need better models? Is eddy-viscosity/eddy-diffusivity assumption good enough?

III. **What is (if it is) preventing LES/WMLES/Hybrid RANS-LES techniques to be routinely used in industrial applications?**
   Robustness, computational cost, proper mesh generation, grey-area (or similar) issues,...

IV. **We can preserve (kinetic) energy. What about other inviscid invariants such as enstrophy (in 2D) or helicity?**

V. **What about time-integration methods?**
   We tend to ignore their effect. Shall we use symplectic time-integration methods?

VI. **Is it possible to preserve linear momentum in multiphase flows?**

