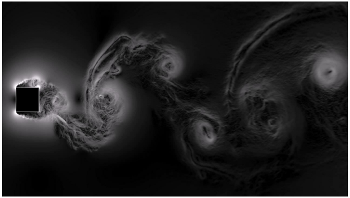
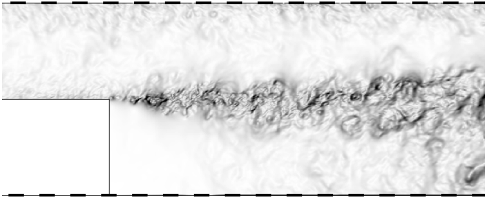
Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

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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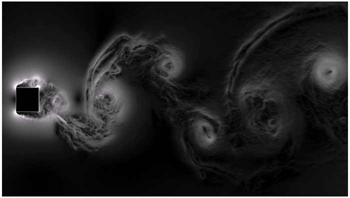

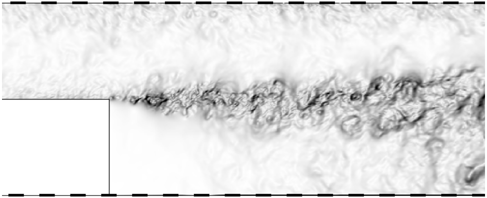

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Preserving symmetries on unstructured grids: paving the way for DNS and LES on complex geometries

F.Xavier Trias

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Contents

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:

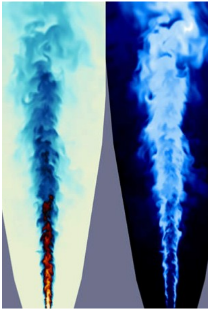
Groningen (2009?)

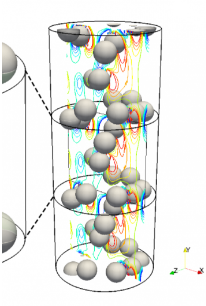
Barcelona (2019)

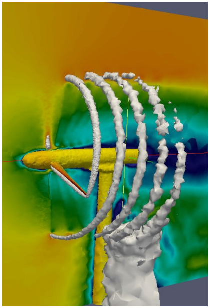
The CTTC research group

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

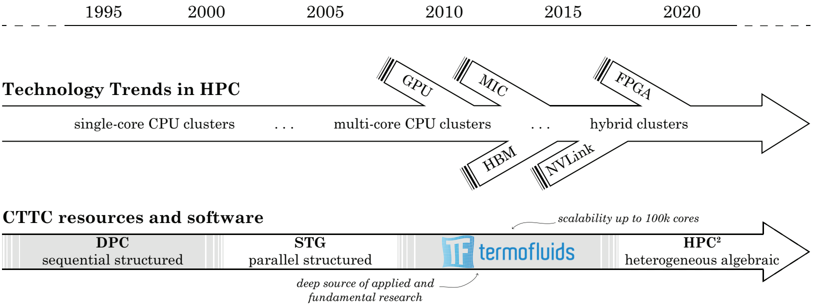
- **Fundamental research** on numerical methods, fluid dynamics and heat and mass transfer phenomena.
- **Applied research** on thermal and fluid dynamic optimization of thermal system and equipment.

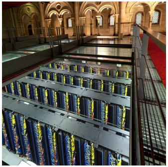


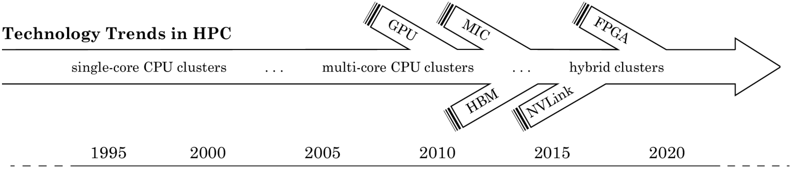


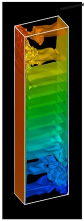


CTTC's historical background in HPC

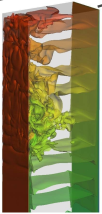




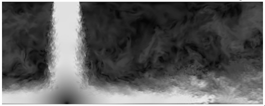




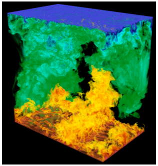
DHC
Ra=10^9
(3.2M)



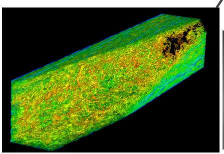
DHC
Ra=10^{11}
(111M)



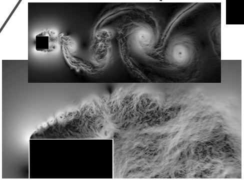
Impinging jet
Re=20000
(102M)



RB
Ra=10^{10} **(607M)**
Ra=10^{11} **(5600M)**



DUCT Re_t=1200 **(172M)**

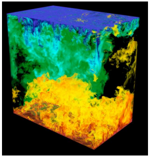


SqCyl Re=22000 **(324M)**

RED ESPAÑOLA DE SUPERCOMPUTACIÓN

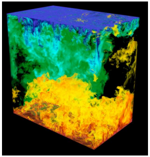
PRACE

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

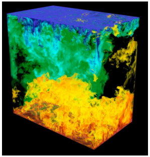
PRACE

intel XEON PLATINUM inside

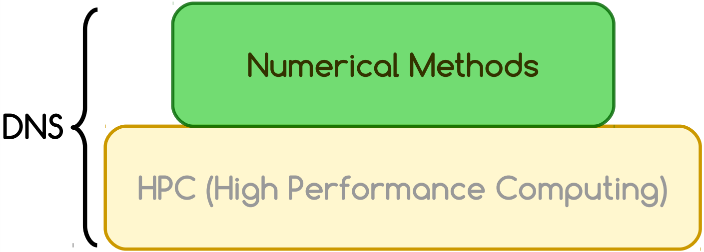
DNS

HPC (High Performance Computing)

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

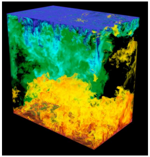


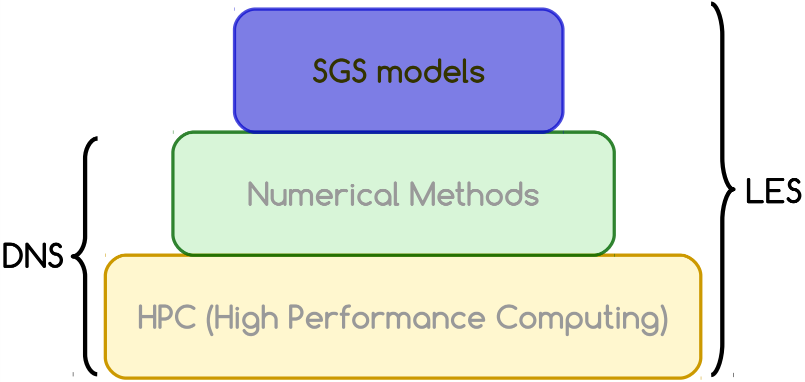
How to properly discretize NS?



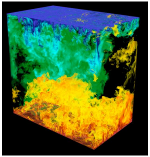
General motivation: (very) large-scale DNS/LES

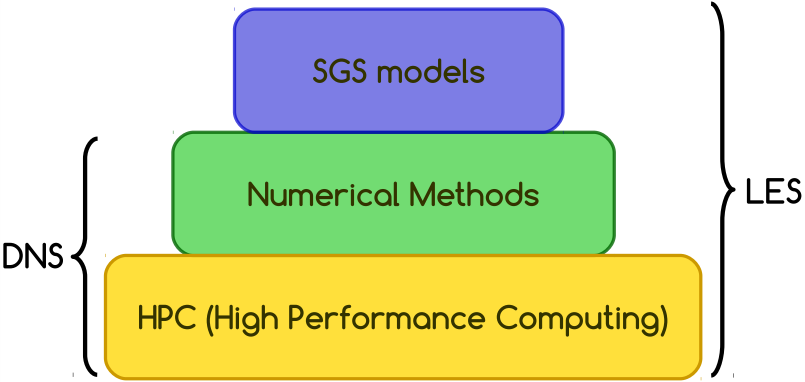
How to properly model SGS?



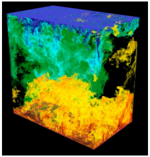


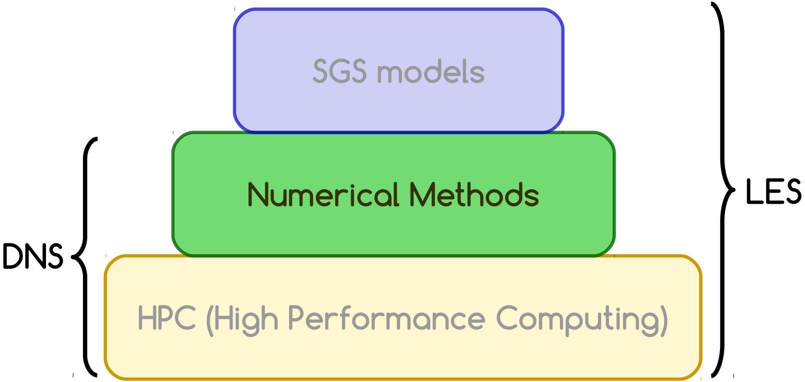
General motivation: (very) large-scale DNS/LES





Numerical methods for DNS/LES

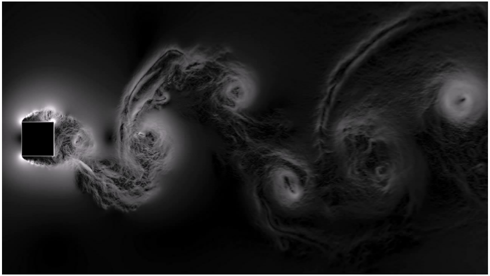


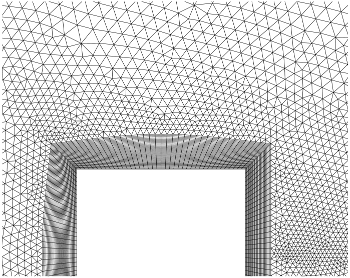


Numerical methods for DNS/LES

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?





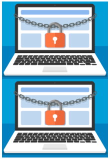
DNS[1] of the turbulent flow around a square cylinder at $Re = 22000$

[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



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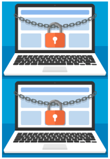
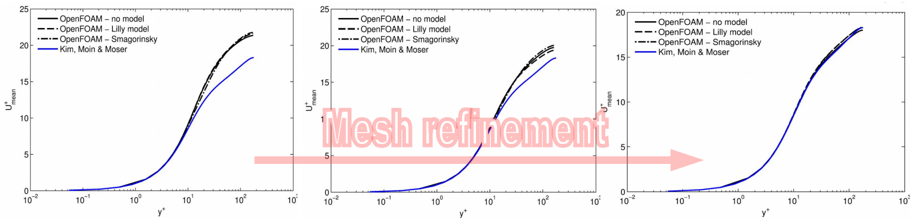


Main common characteristics of LES in such codes:

- **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 $Re_\tau = 180$



$13 \times 76 \times 20$ — $\Delta x^+ = 90, \Delta y^+_{wall} = 0.5, \Delta z^+ = 30$

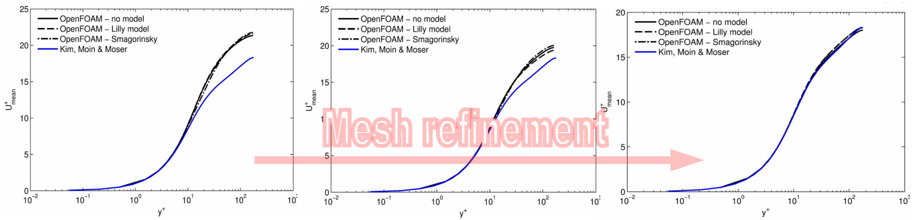
$19 \times 78 \times 28$ — $\Delta x^+ = 60, \Delta y^+_{wall} = 0.5, \Delta z^+ = 20$

$38 \times 78 \times 57$ — $\Delta x^+ = 30, \Delta y^+_{wall} = 0.5, \Delta z^+ = 10$

[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

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



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

- 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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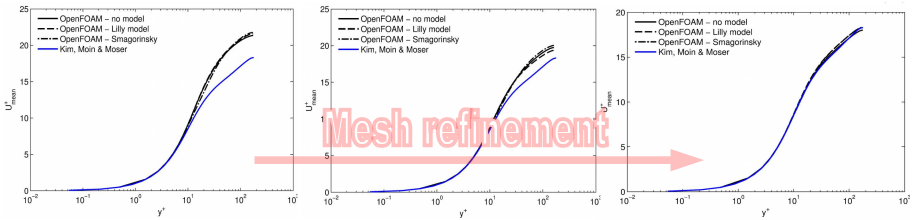


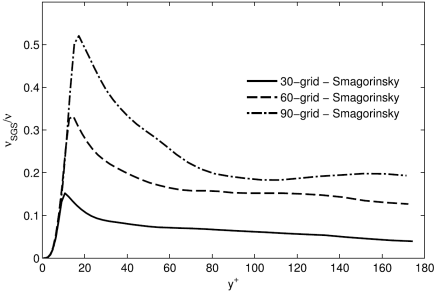
13×76×20	19×78×28	38×78×57
$\Delta x^+ = 90, \Delta y^+_{wall} = 0.5, \Delta z^+ = 30$	$\Delta x^+ = 60, \Delta y^+_{wall} = 0.5, \Delta z^+ = 20$	$\Delta x^+ = 30, \Delta y^+_{wall} = 0.5, \Delta z^+ = 10$

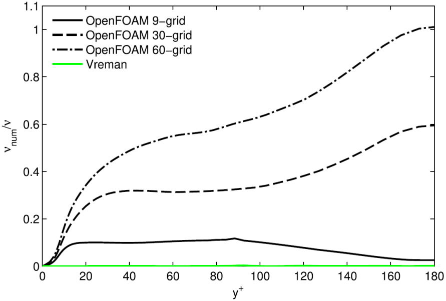
- Are LES results are merit of the SGS model? Apparently **NOT**!!! ✗

[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.

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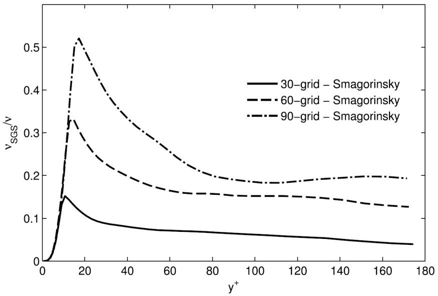
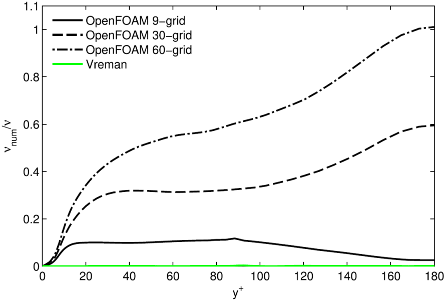




$$\nu_{SGS} < \nu_{num} \neq 0$$

[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

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

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

Symmetry-preserving discretization

Continuous

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

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

Discrete

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

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

Symmetry-preserving discretization

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

Symmetry-preserving discretization

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

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

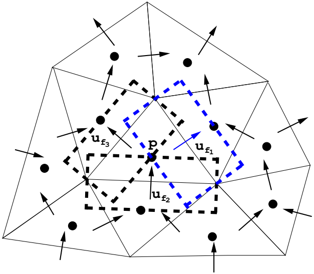
Why collocated arrangements are so popular?

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

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

In <u>staggered meshes</u>

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



Why collocated arrangements are so popular?

- STAR-CCM+
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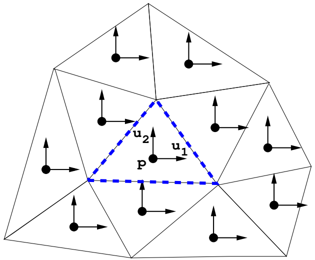
- OpenFOAM

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

In <u>collocated meshes</u>

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



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 — Open∇FOAM®, GPL v3 Free Software

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

In <u>collocated meshes</u>

- p-$\boldsymbol{u}_c$ coupling is cumbersome ✗
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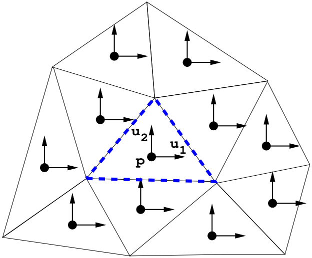

Pressure-velocity coupling on collocated grids

A vicious circle that cannot be broken...

In summary[5]:

- Mass: $\mathsf{M}\Gamma_{c\rightarrow s}\boldsymbol{u}_c = \mathsf{M}\Gamma_{c\rightarrow s}\boldsymbol{u}_c - \mathsf{L}_c\mathsf{L}^{-1}\mathsf{M}\Gamma_{c\rightarrow s}\boldsymbol{u}_c \approx \boldsymbol{0}_c$ ✗
- Energy: $\boldsymbol{p}_c\left(\mathsf{L}-\mathsf{L}_c\right)\boldsymbol{p}_c \neq 0$ ✗

[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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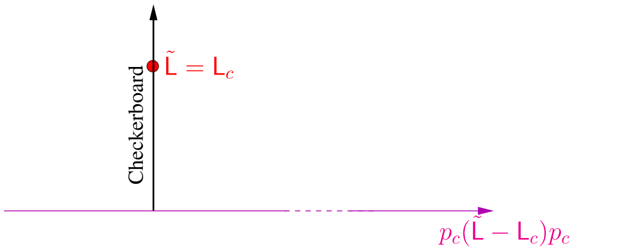

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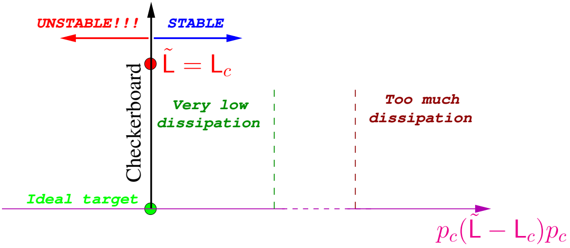

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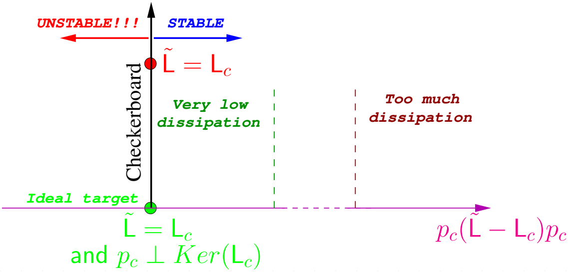

[5] Shashank, J.Larsson, G.Iaccarino. *A co-located incompressible Navier-Stokes solver with exact mass, momentum and kinetic energy conservation in the inviscid limit*, **Journal of Computational Physics**, 229: 4425-4430,2010.

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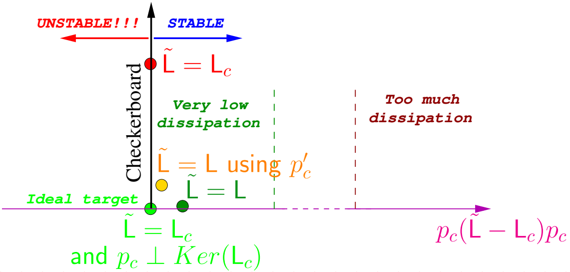

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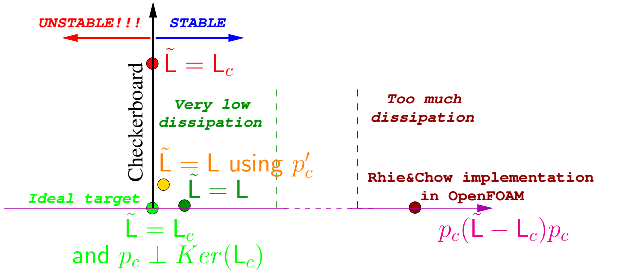

[5] E.Komen, J.A.Hopman, E.M.A.Frederix, F.X.Trias, R.W.C.P.Verstappen. "A symmetry-preserving second-order time-accurate PISO-based method". **Computers & Fluids**, 225:104979, 2021. (github.com/janneshopman)

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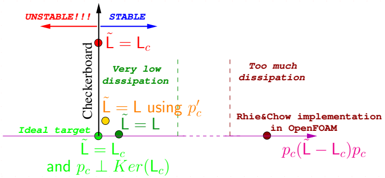

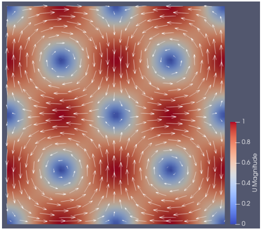

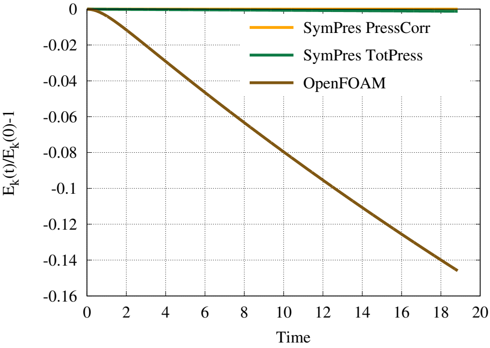

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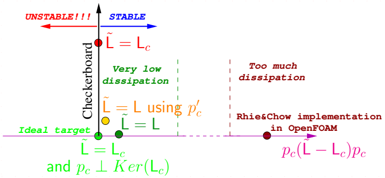

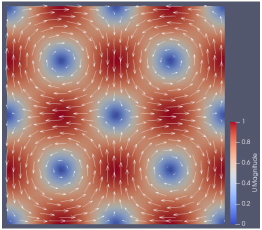

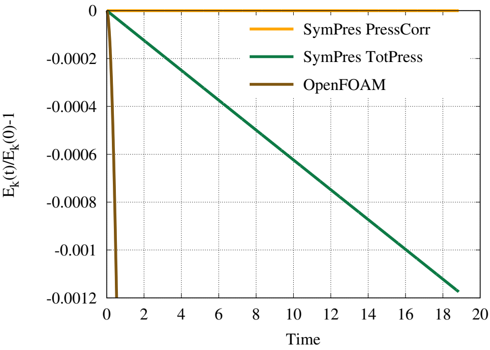

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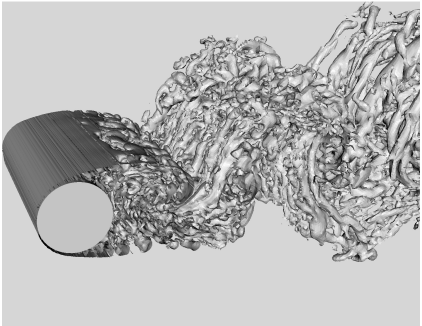
Pressure-velocity coupling on collocated grids

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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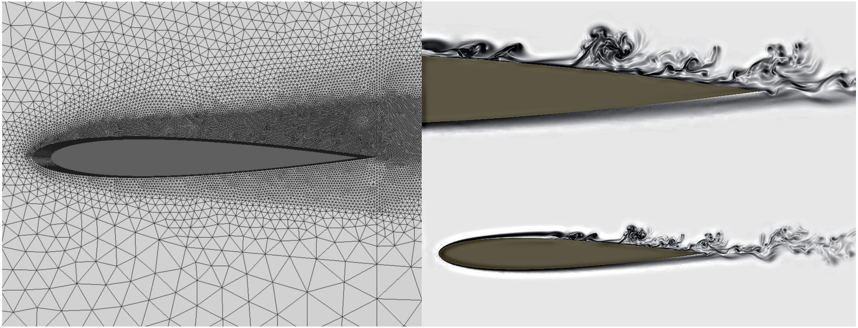
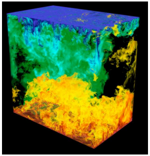
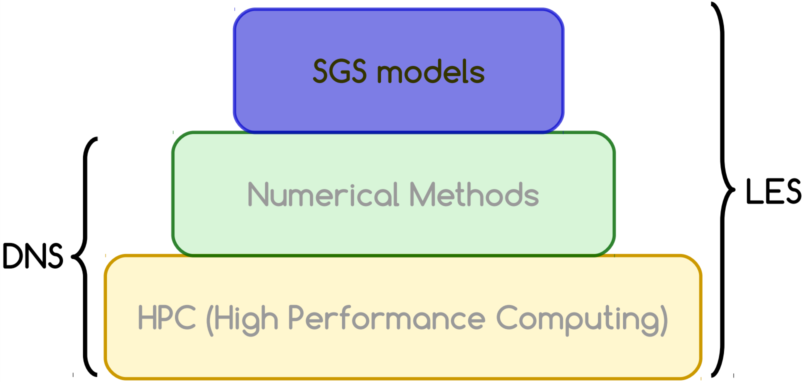


[7] F.X.Trias and O.Lehmkuhl. *A self-adaptive strategy for the time-integration of Navier-Stokes equations*. **Numerical Heat Transfer, part B**, 60(2):116-134, 2011.

LES of RBC

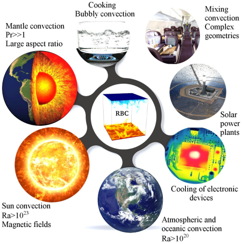


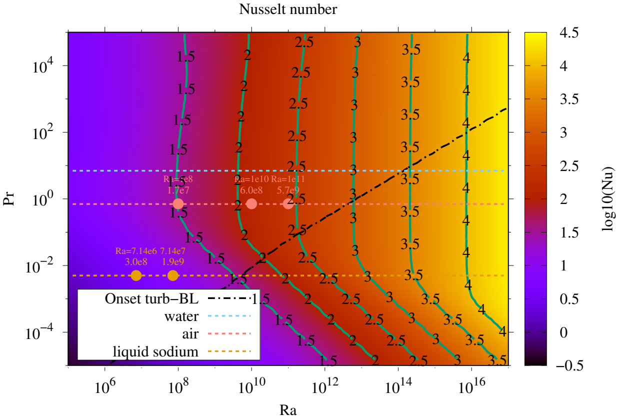

SGS models
Numerical Methods
HPC (High Performance Computing)
DNS
LES

LES of RBC

Research question #2:

- Can we hit the ultimate regime of thermal turbulence ?





LES of RBC

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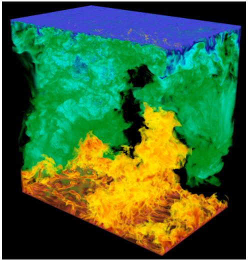

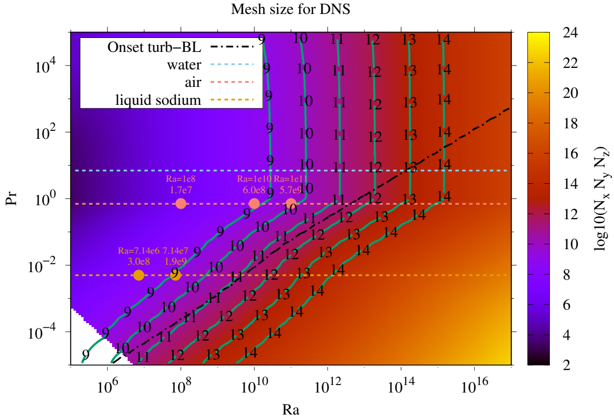

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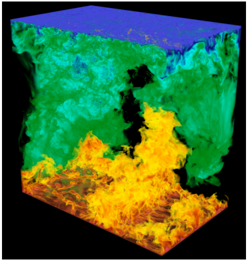

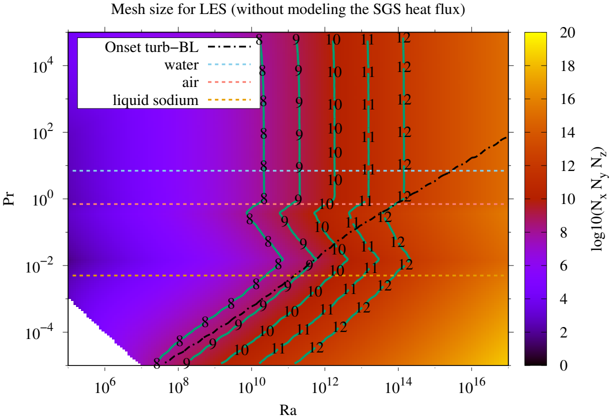

Problems to model the SGS heat flux[8]

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

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

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eddy-diffusivity

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

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

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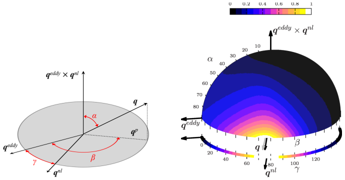

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DNS results at very low Pr number

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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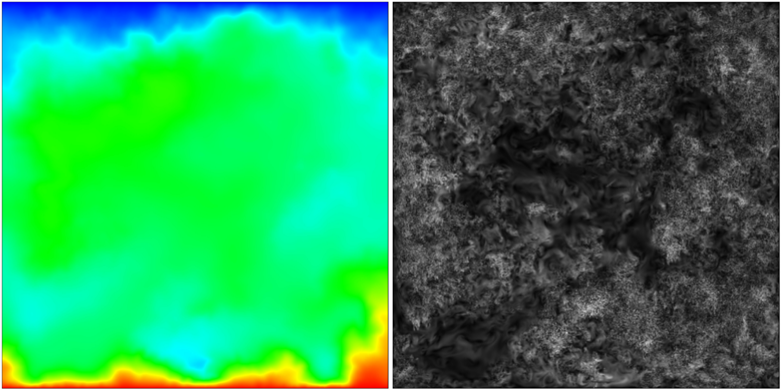

DNS of a RB at $Ra = 7.14 \times 10^6$ and $Pr = 0.005$ (liquid sodium)

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

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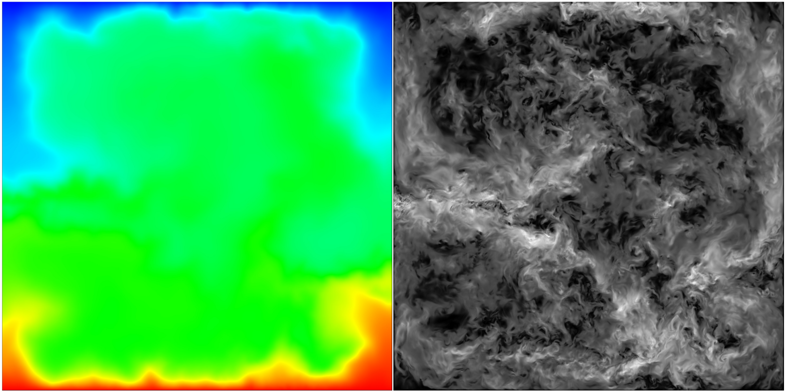

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$966 \times 966 \times 2048 \approx$ **1911M**

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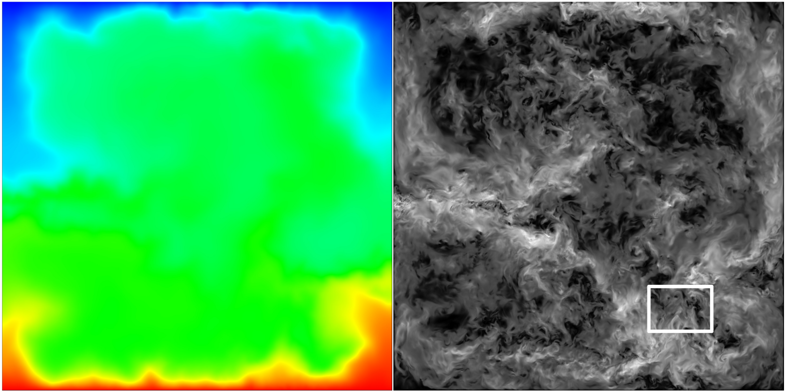

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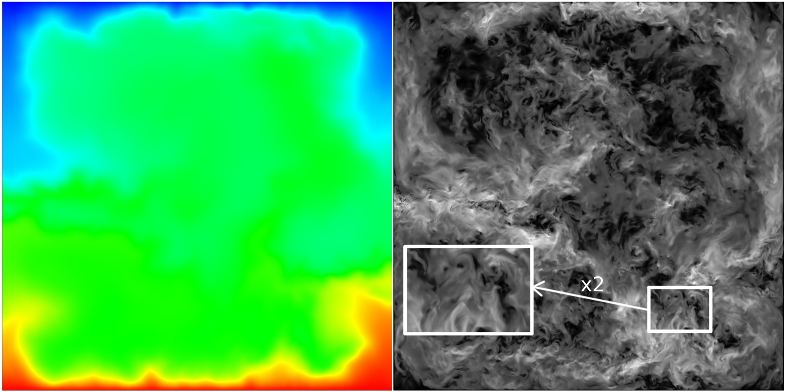

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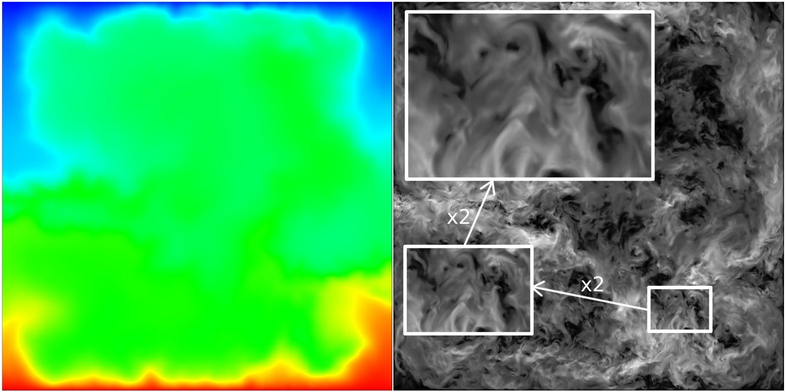

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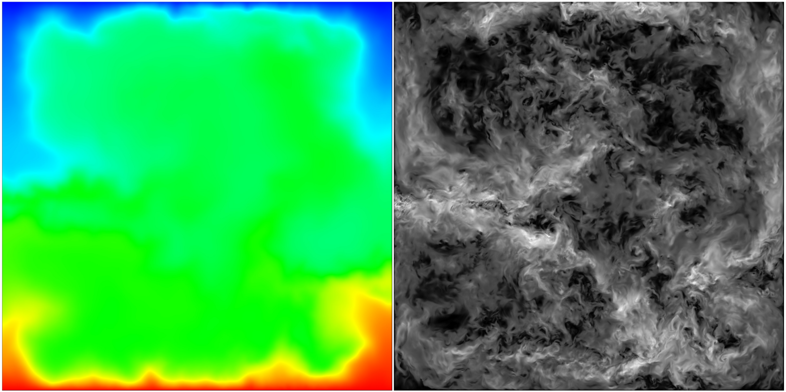
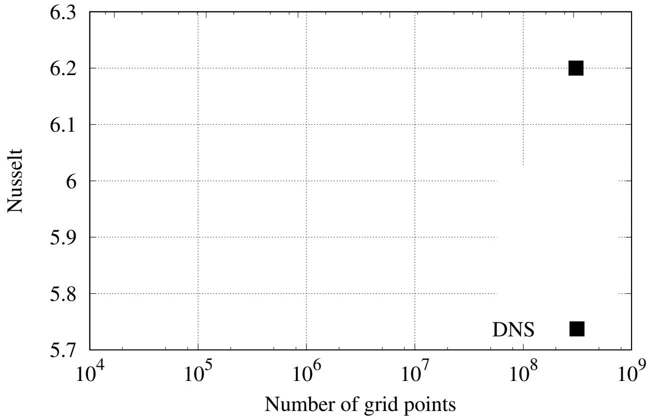


DNS of a RB at $Ra = 7.14 \times 10^7$ and $Pr = 0.005$ (liquid sodium)

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

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

RB at $\boxed{Ra = 7.14 \times 10^6}$ and $Pr = 0.005$ (DNS $\rightarrow 488 \times 488 \times 1280 \approx$ **305M**)



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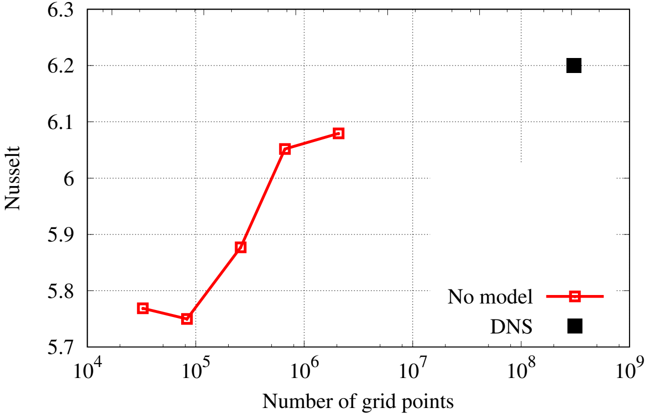

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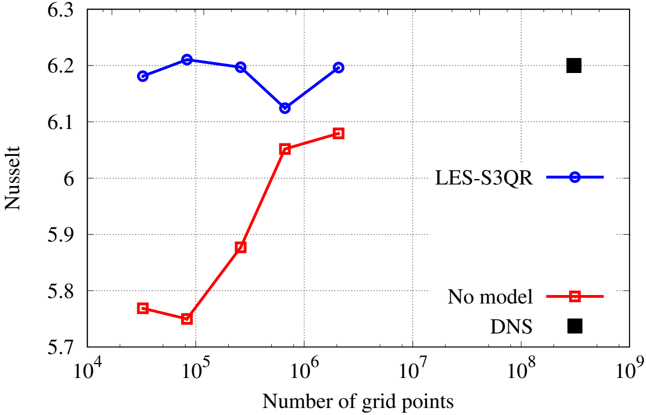

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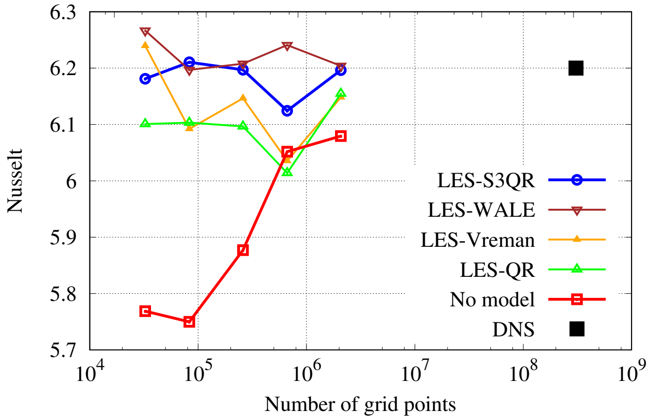

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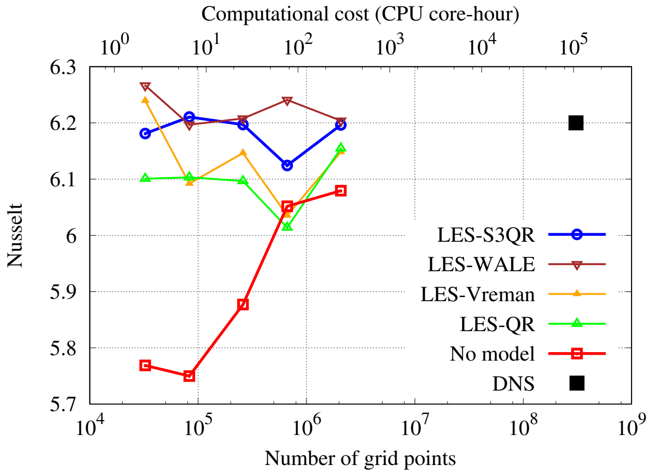

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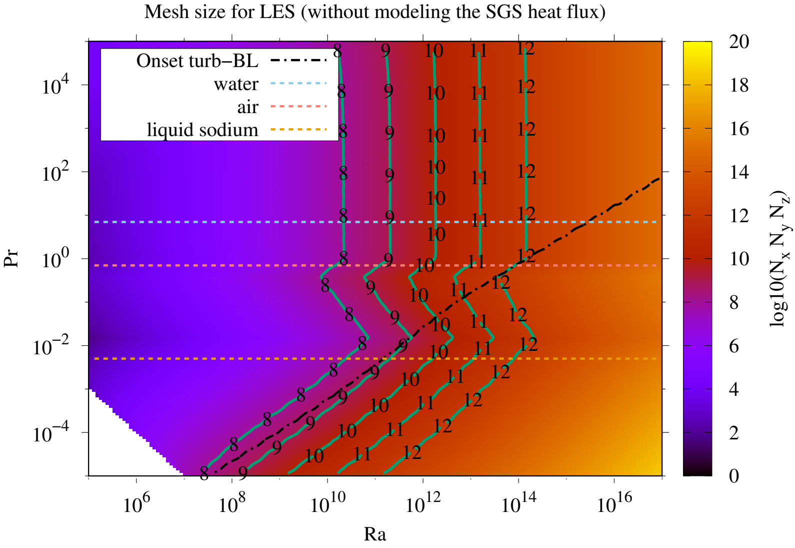

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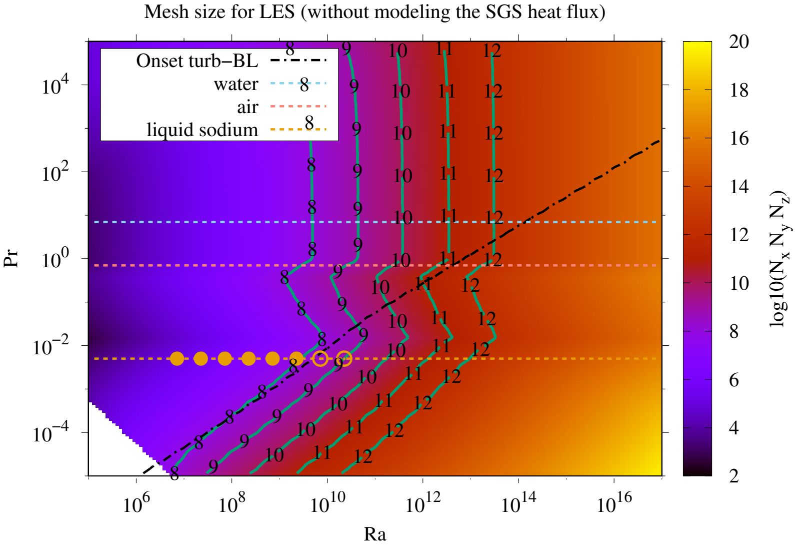

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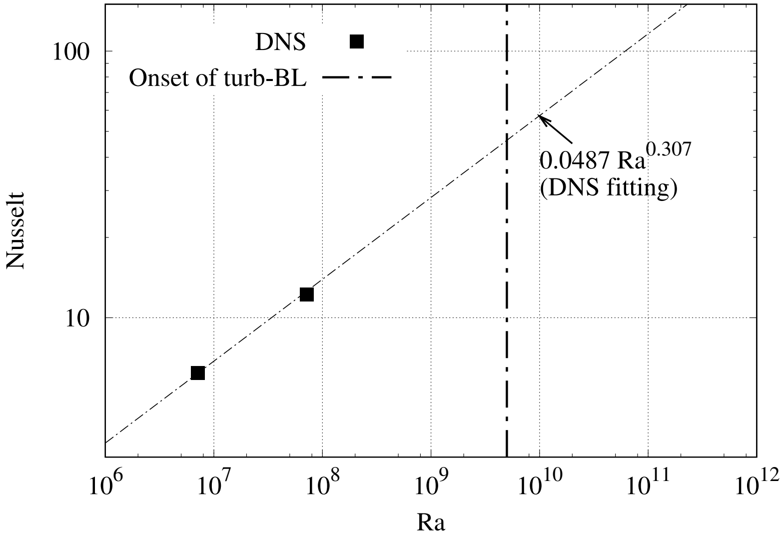

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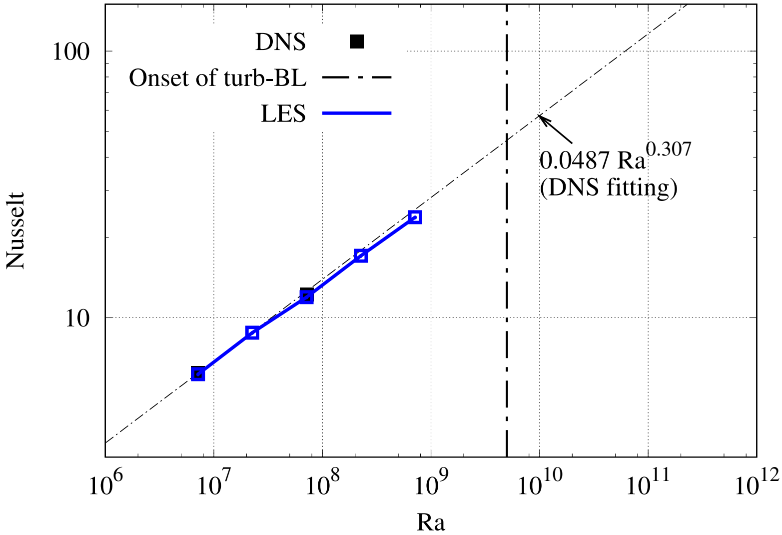

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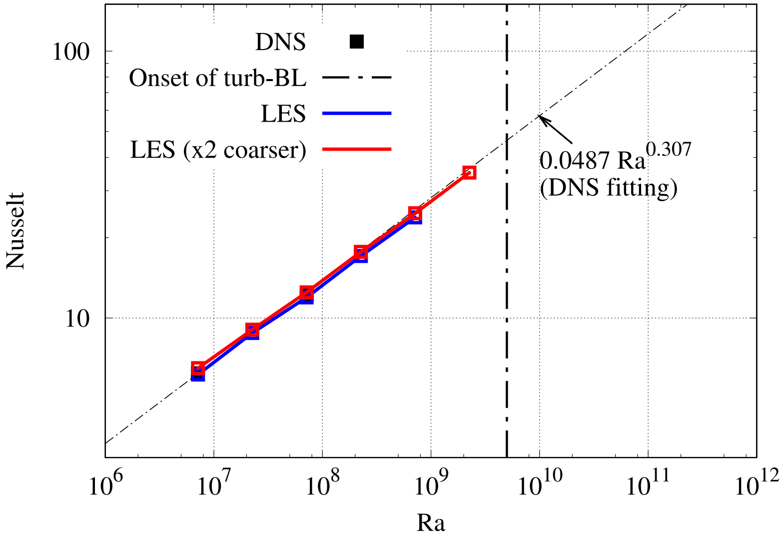
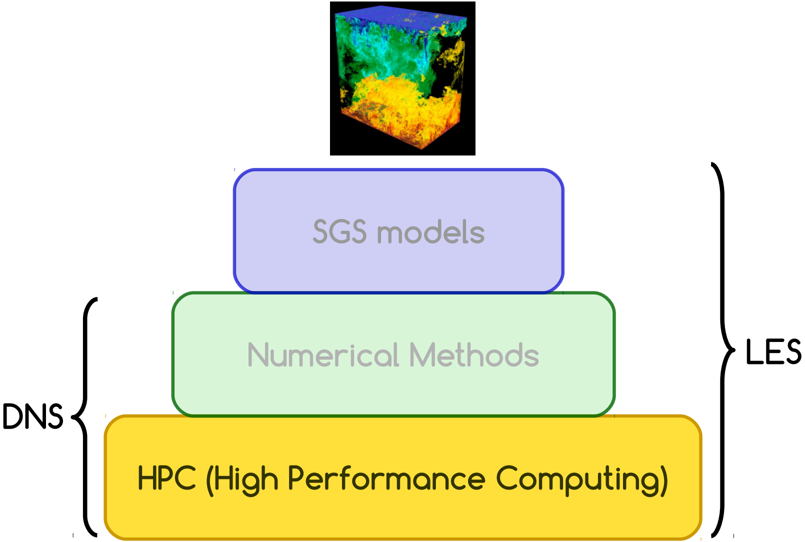


HPC on modern supercomputers



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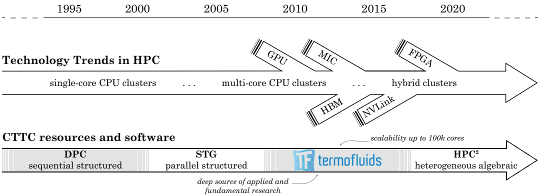
Research question #3:

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



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[10] X.Álvarez, A.Gorobets, F.X.Trias, R.Borrell, and G.Oyarzun. *HPC^2 - a fully portable algebra-dominant framework for heterogeneous computing. Application to CFD*. **Computers & Fluids**, 173:285-292, 2018

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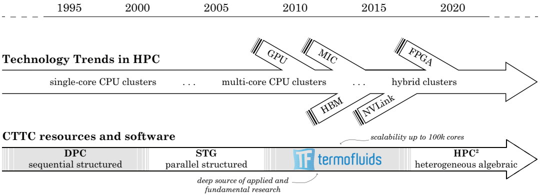

HPC^2: portable, algebra-based framework for heterogeneous computing is being developed[10]. Traditional stencil-based data and sweeps are replaced by algebraic structures (sparse matrices and vectors) and kernels. `SpMM`-based strategies to increase the arithmetic intensity are under development[11].

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

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

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

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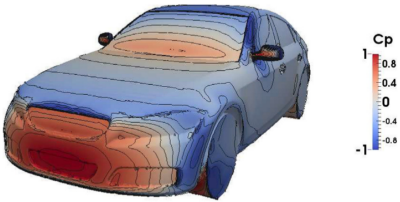
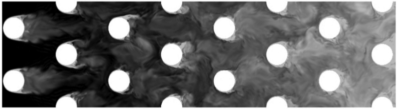
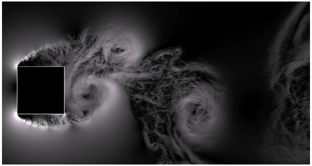
Minimal set of kernels:

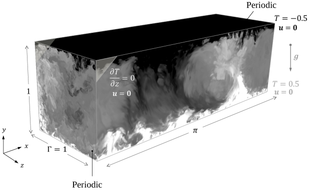
$$\begin{aligned} \texttt{SpMM}: &\quad \boldsymbol{y} \leftarrow A\boldsymbol{x} \\ \texttt{axpy}: &\quad \boldsymbol{z} \leftarrow a\boldsymbol{x} + b\boldsymbol{y} \\ \texttt{dot}: &\quad r \leftarrow \boldsymbol{x} \cdot \boldsymbol{y} \end{aligned}$$

Algebra-based approach naturally leads to portability, to simple and analyzable formulations and opens the door to new strategies[12] to improve its perfomance...









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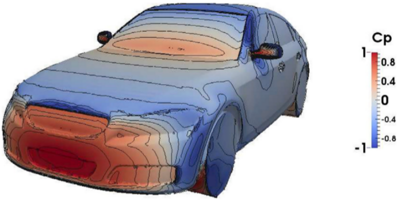
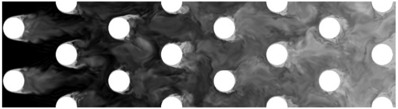
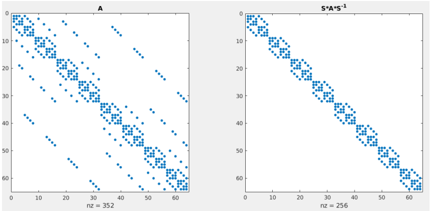




$$\hat{\mathsf{L}} = \mathsf{S}\mathsf{L}\mathsf{S}^{-1} = \mathsf{I} \otimes \mathsf{L}_{inn} + diag(\boldsymbol{d})$$



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

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- Higher arithmetic intensity (AI)
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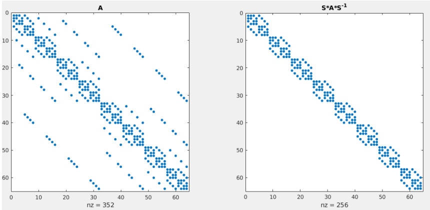

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→ Overall speed-up up to **x2-x3** ✓
→ Memory reduction of ≈**2** ✓

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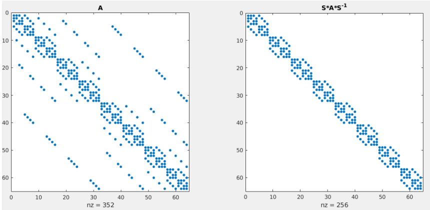

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Other SpMM-based strategies to **increase AI** and **reduce memory** footprint:

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

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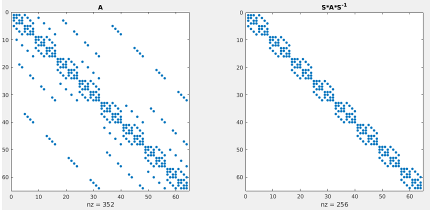

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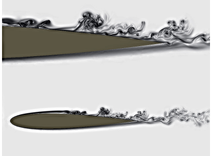
- **Preserving symmetries** either using staggered or collocated formulations is the key point for **reliable LES/DNS** simulations.



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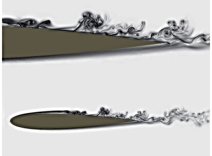

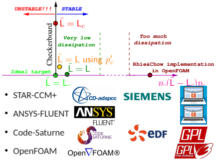

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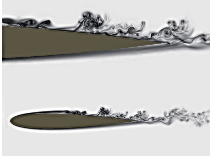
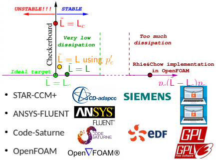
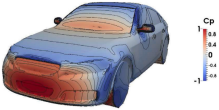
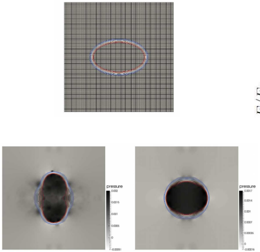


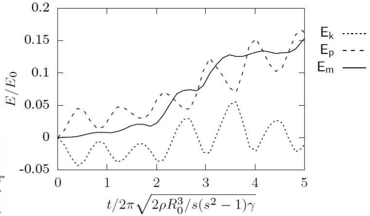




On-going (related) research

- **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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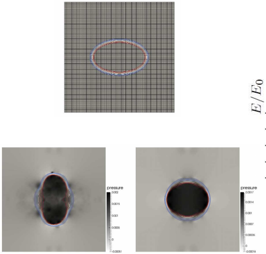

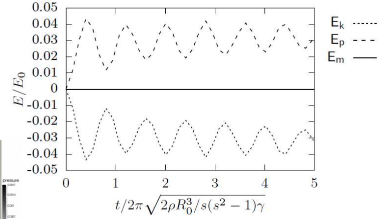

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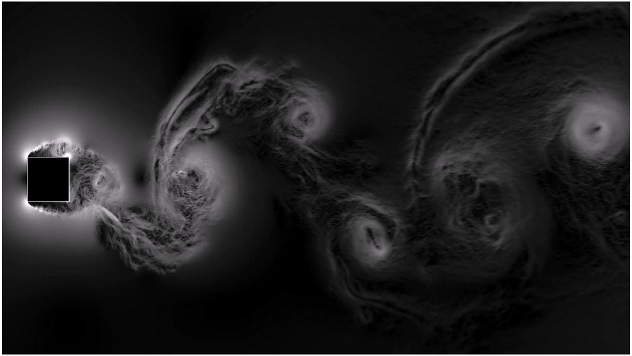
Thank you for your attendance



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?**