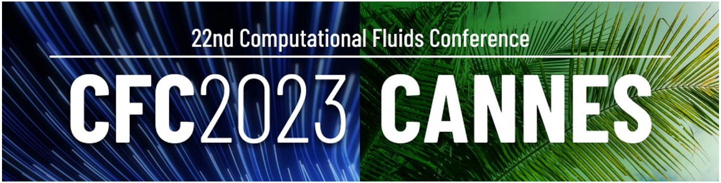
Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

An energy-preserving unconditionally stable method for DNS and LES simulations on unstructured grids

F.Xavier Trias[1], Daniel Santos[1], Jannes Hopman[1], Andrey Gorobets[2], Assensi Oliva[1]

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



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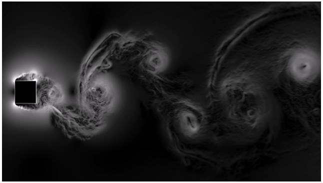
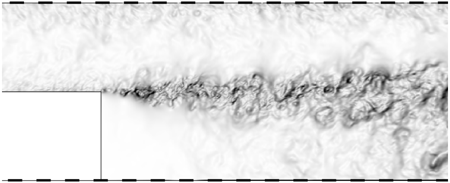


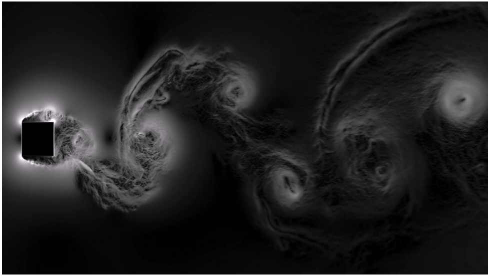


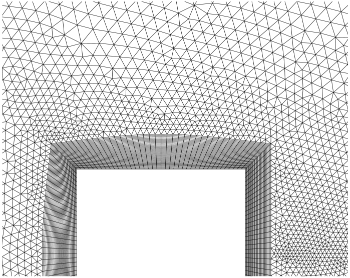
Contents

Motivation

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?





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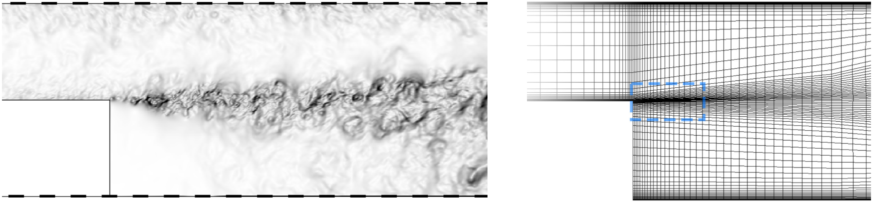

DNS[2] of backward-facing step at $Re_\tau = 395$ and expansion ratio 2

[2] A.Pont-Vílchez, F.X.Trias, A.Gorobets, A.Oliva. *DNS of Backward-Facing Step flow at $Re_\tau = 395$ and expansion ratio 2*. **Journal of Fluid Mechanics**, 863:341-363, 2019.

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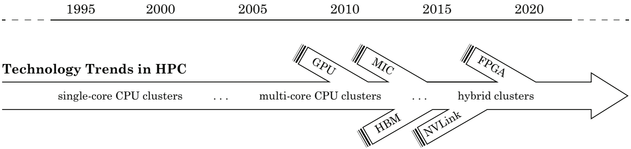
Research question #2:

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



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

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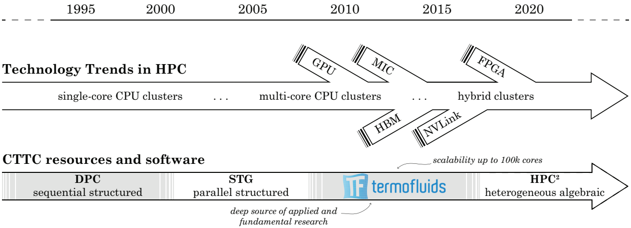

HPC²: portable, algebra-based framework for heterogeneous computing is being developed[3]. Traditional stencil-based data and sweeps are replaced by algebraic structures (sparse matrices and vectors) and kernels. SpMM-based strategies to increase the arithmetic intensity are being considered[4].

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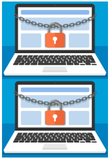
Frequently used general purpose CFD codes:

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



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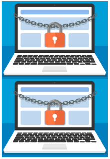
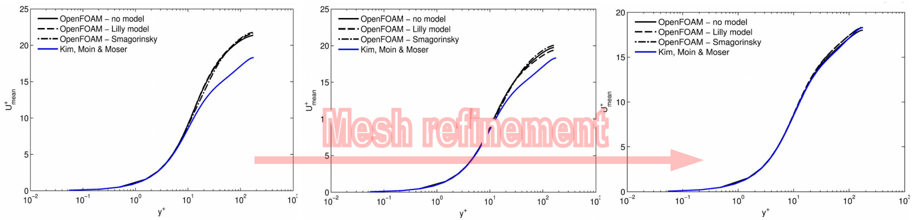


Main common characteristics of LES in such codes:

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

Motivation

Open∇FOAM® LES[5] results of a turbulent channel for at $Re_\tau = 180$



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

[5] 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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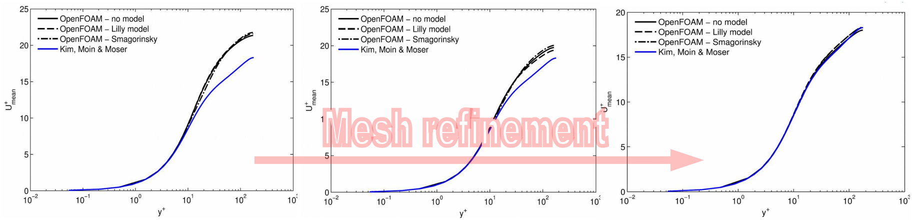

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- Are LES results are merit of the SGS model?

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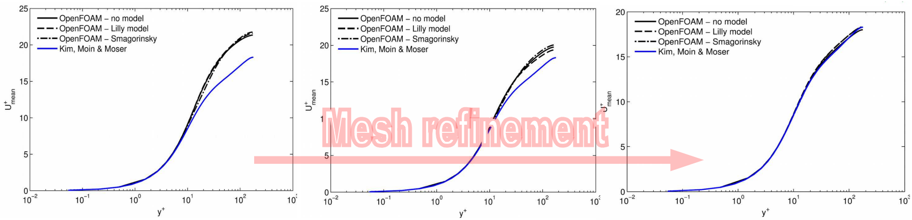

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- Are LES results are merit of the SGS model? Apparently **NOT**!!! ✗

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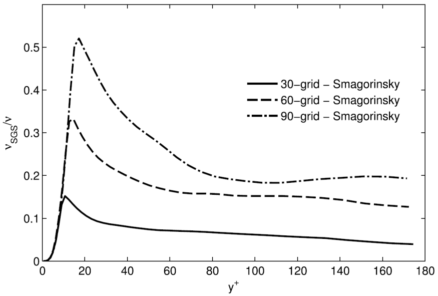
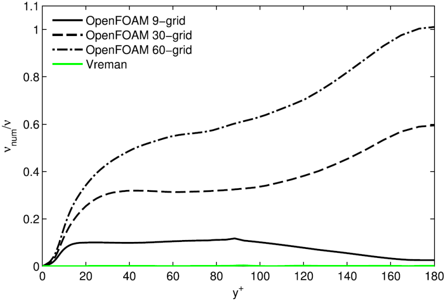
OpenFOAM® LES[6] results of a turbulent channel for at $Re_\tau = 180$





$\nu_{num} \neq 0$

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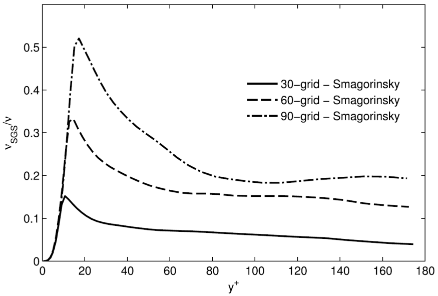

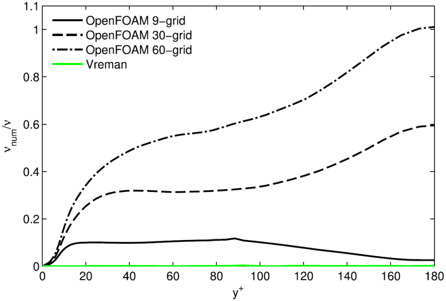

$$\nu_{SGS} < \nu_{num} \neq 0$$

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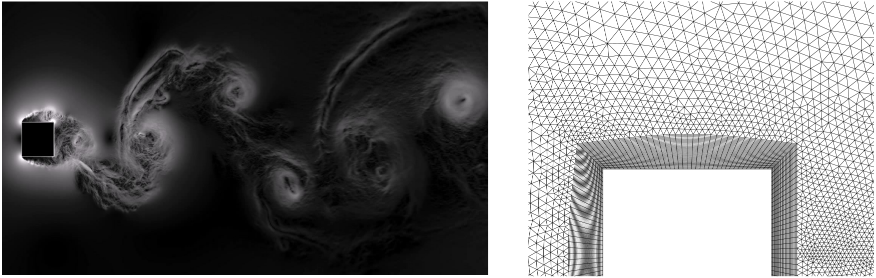

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Symmetry-preserving discretization

Continuous

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

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

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

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Discrete

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

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

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

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$\langle C(\mathbf{u}, \varphi_1), \varphi_2 \rangle = -\langle C(\mathbf{u}, \varphi_2), \varphi_1 \rangle$	$\mathsf{C}(\mathbf{u}_h) = -\mathsf{C}^T(\mathbf{u}_h)$

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

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

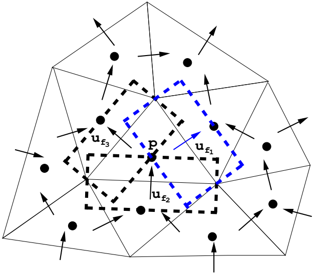
Why collocated arrangements are so popular?

- STAR-CCM+ — CD-adapco, SIEMENS
- ANSYS-FLUENT — ANSYS FLUENT®
- Code-Saturne — CODE SATURNE, eDF, GPL
- OpenFOAM — Open∇FOAM®, GPLv3 Free Software

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

In staggered meshes

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



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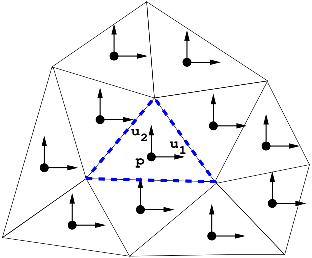
In collocated meshes

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



Why collocated arrangements are so popular?

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

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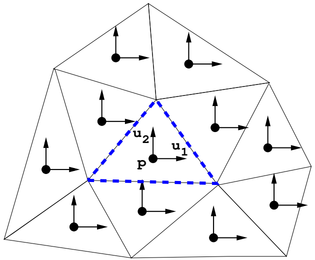

Pressure-velocity coupling on collocated grids

A vicious circle that cannot be broken...

In summary[7]:

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

[7] 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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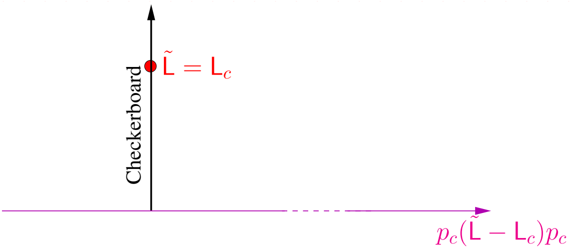

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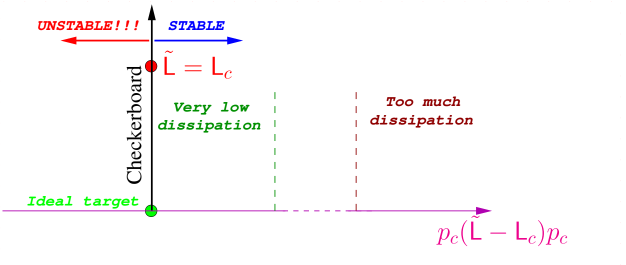

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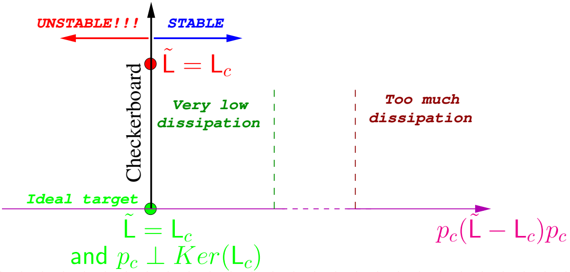

[7]Shashank, J.Larsson, G.Iaccarino. *A co-located incompressible Navier-Stokes solver with exact mass, momentum and kinetic energy conservation in the inviscid limit*, **Journal of Computational Physics**, 229: 4425-4430,2010.

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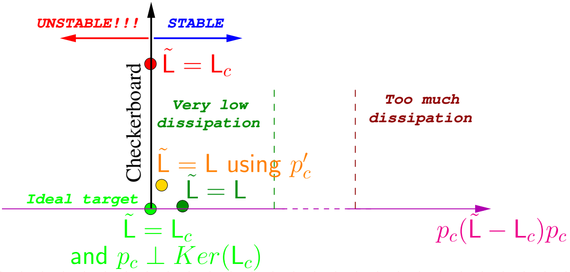

[7] F.X.Trias, O.Lehmkuhl, A.Oliva, C.D.Pérez-Segarra, R.W.C.P.Verstappen. *Symmetry-preserving discretization of Navier-Stokes equations on collocated unstructured grids*, **Journal of Computational Physics**, 258 (1): 246-267, 2014.

Pressure-velocity coupling on collocated grids

A vicious circle that cannot be broken...

In summary[7]:

- Mass: $\mathsf{M}\Gamma_{c\rightarrow s}\boldsymbol{u}_c = \mathsf{M}\Gamma_{c\rightarrow s}\boldsymbol{u}_c - \mathsf{L}_c\mathsf{L}^{-1}\mathsf{M}\Gamma_{c\rightarrow s}\boldsymbol{u}_c \approx \mathbf{0}_c$ ✗
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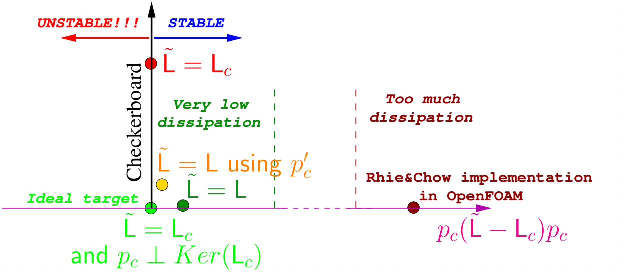

[7] E.Komen, J.A.Hopman, E.M.A.Frederix, F.X.Trias, R.W.C.P.Verstappen. "A symmetry-preserving second-order time-accurate PISO-based method". **Computers & Fluids**, 225:104979, 2021.

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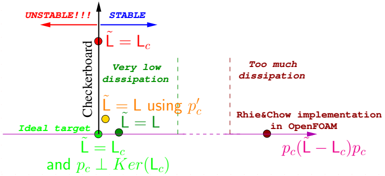

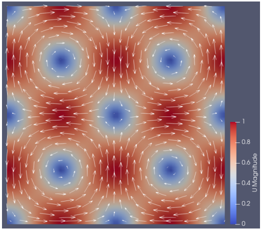

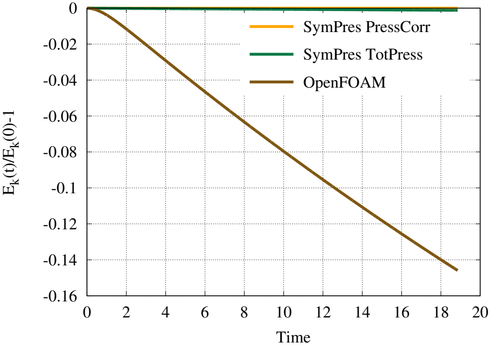

Results for an inviscid Taylor-Green vortex[8]

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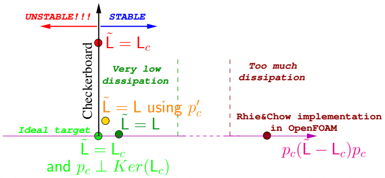

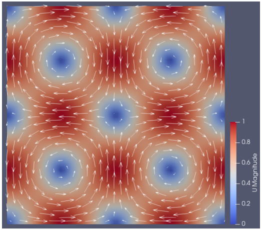

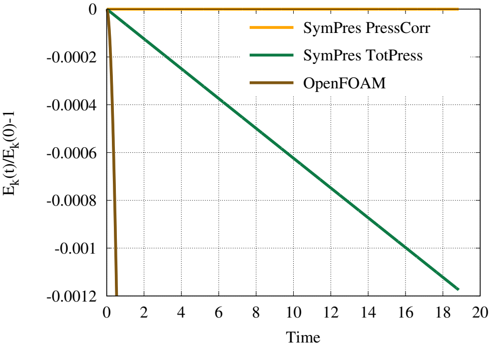

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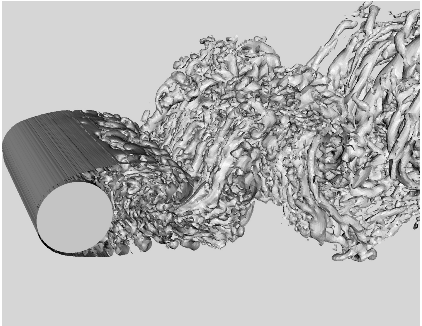
Pressure-velocity coupling on collocated grids

Examples of simulations

Despite these inherent limitations, symmetry-preserving collocated formulation has been successfully used for DNS/LES simulations[9]:



[9] 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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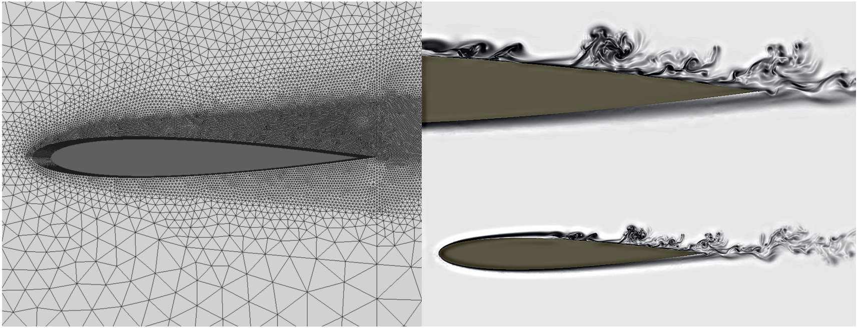
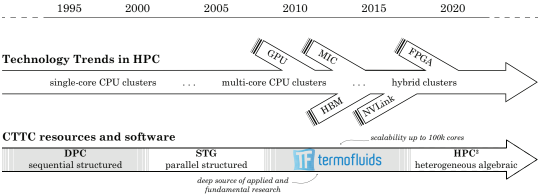


[9] F.X.Trias and O.Lehmkuhl. *A self-adaptive strategy for the time-integration of Navier-Stokes equations*. **Numerical Heat Transfer, part B**, 60(2):116-134, 2011.

Algebra-based approach naturally leads to portability

Research question #2:

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



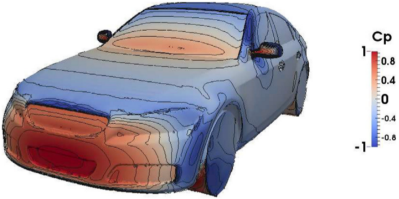
HPC^2: portable, algebra-based framework for heterogeneous computing is being developed. Traditional stencil-based data and sweeps are replaced by algebraic structures (sparse matrices and vectors) and kernels. `SpMM`-based strategies to increase the arithmetic intensity are being considered[10].

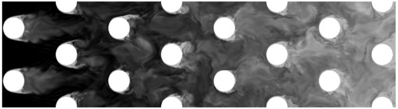
[10] À.Alsalti-Baldellou, X.Álvarez-Farré, F.X.Trias, A.Oliva. *Exploiting spatial symmetries for solving Poisson's equation*. **Journal of Computational Physics**, 486:112133, 2023.

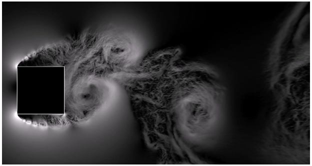
Algebra-based approach naturally leads to portability, to simple and analyzable formulations

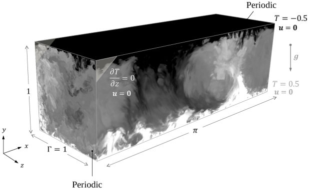
Continuous	Discrete
$\frac{\partial \boldsymbol{u}}{\partial t} + C(\boldsymbol{u}, \boldsymbol{u}) = \nu \nabla^2 \boldsymbol{u} - \nabla p$	$\Omega \frac{d\boldsymbol{u}_h}{dt} + \mathsf{C}(\boldsymbol{u}_h)\boldsymbol{u}_h = \mathsf{D}\boldsymbol{u}_h - \mathsf{G}\boldsymbol{p}_h$
$\nabla \cdot \boldsymbol{u}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

Algebra-based approach naturally leads to portability, to simple and analyzable formulations and opens the door to new strategies[11] to improve its perfomance...









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

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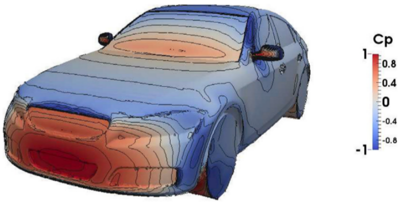
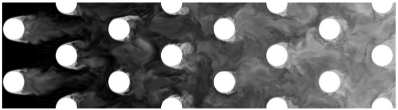
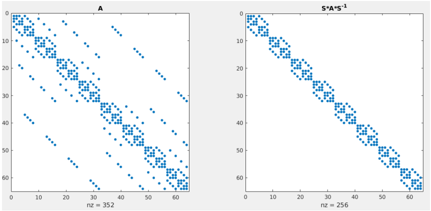




$$\hat{L} = SLS^{-1} = I \otimes L_{inn} + diag(\boldsymbol{d})$$



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- Higher arithmetic intensity (AI)
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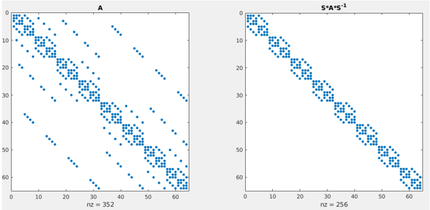

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→ Overall speed-up up to **x2-x3** ✓
→ Memory reduction of ≈**2** ✓

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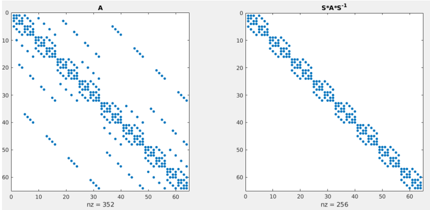

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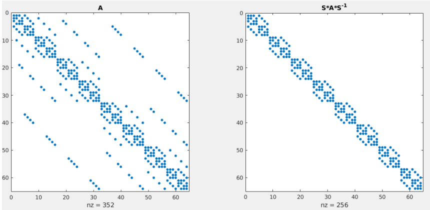
Other SpMM-based strategies to **increase AI** and **reduce memory** footprint:

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

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



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Concluding remarks

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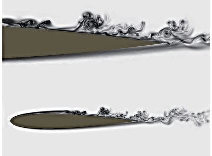

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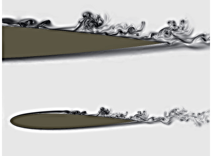

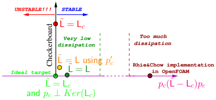

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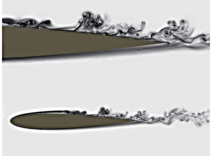

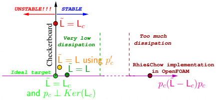

On-going research:

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

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Thank you for your attendance