



Centre Tecnològic de Transferència de Calor  
UNIVERSITAT POLITÈCNICA DE CATALUNYA



# Preserving operator symmetries on unstructured grids

F.Xavier Trias<sup>1</sup>, Xavier Álvarez<sup>1</sup>, Andrey Gorobets<sup>2</sup>, Assensi Oliva<sup>1</sup>

<sup>1</sup>Heat and Mass Transfer Technological Center, Technical University of Catalonia

<sup>2</sup>Keldysh Institute of Applied Mathematics of RAS, Russia



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

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**HiFiLeD** SYMPOSIUM

2nd High-Fidelity Industrial LES/DNS Symposium  
*Paving the way for future accurate CFD*

22-24 September 2021  
(online event)

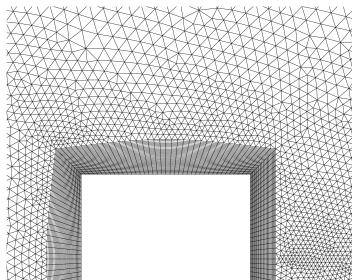
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- 2 Preserving symmetries at discrete level
- 3 Portability and beyond
- 4 Conclusions

# 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?



DNS<sup>1</sup> of the turbulent flow around a square cylinder at  $Re = 22000$

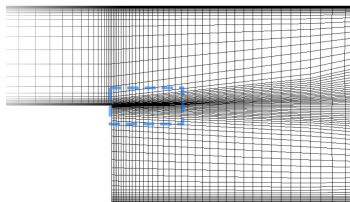
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<sup>1</sup>F.X.Trias, A.Gorobets, A.Oliva. *Turbulent flow around a square cylinder at Reynolds number 22000: a DNS study*, **Computers&Fluids**, 123:87-98, 2015.

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DNS<sup>2</sup> of backward-facing step at  $Re_\tau = 395$  and expansion ratio 2

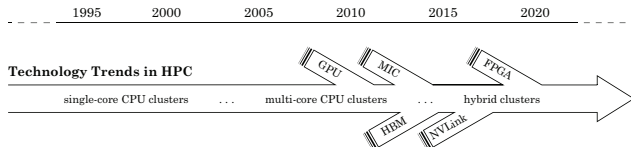
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<sup>2</sup>A.Pont-Vílchez, F.X.Trias, A.Gorobets, A.Oliva. *DNS of Backward-Facing Step flow at  $Re_\tau = 395$  and expansion ratio 2*. **Journal of Fluid Mechanics**, 863:341-363, 2019.

# Motivation

## Research question #2:

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



<sup>3</sup>X.Álvarez, A.Gorobets, F.X.Trias, R.Borrell, and G.Oyarzun. *HPC<sup>2</sup> - a fully portable algebra-dominant framework for heterogeneous computing. Application to CFD*. **Computers & Fluids**, 173:285-292, 2018

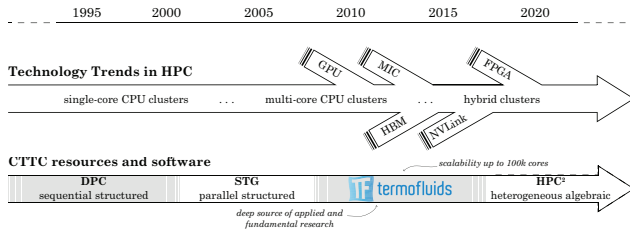
<sup>4</sup>X.Álvarez, A.Gorobets, F.X.Trias. *A hierarchical parallel implementation for heterogeneous computing. Application to algebra-based CFD simulations on hybrid supercomputers*. **Computers & Fluids**, 214:104768, 2021.

<sup>5</sup>X.Álvarez-Farré, À.Alsalti-Baldellou, A.Gorobets, A.Oliva, F.X.Trias. *Enabling larger and faster simulations from mesh symmetries*. **HiFiLeD2 Symposium** Don't miss it!

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



**HPC<sup>2</sup>:** portable, algebra-based framework<sup>3</sup> for heterogeneous computing is being developed<sup>4</sup>. 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 presented in this Symposium<sup>5</sup>.






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# Motivation

Frequently used general purpose CFD codes:

- STAR-CCM+  **SIEMENS** 
- ANSYS-FLUENT 
- Code-Saturne  **edf** 
- OpenFOAM  



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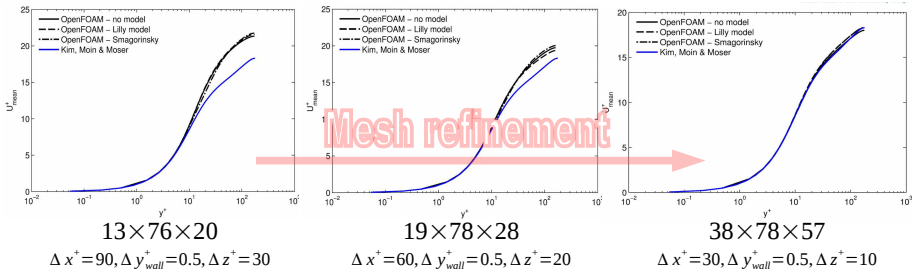
- STAR-CCM+  **SIEMENS** 
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Main common characteristics of LES in such codes:

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

# Motivation

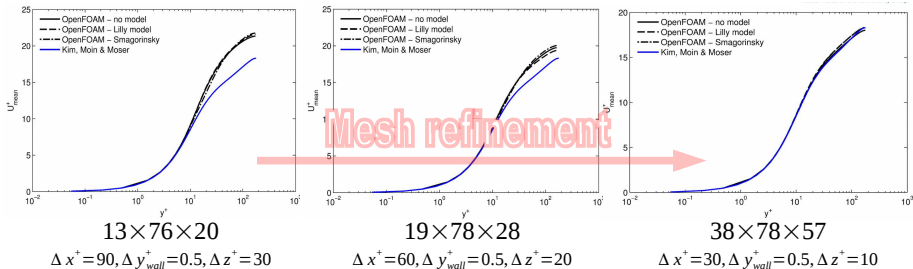
OpenFOAM® LES<sup>6</sup> results of a turbulent channel for at  $Re_\tau = 180$



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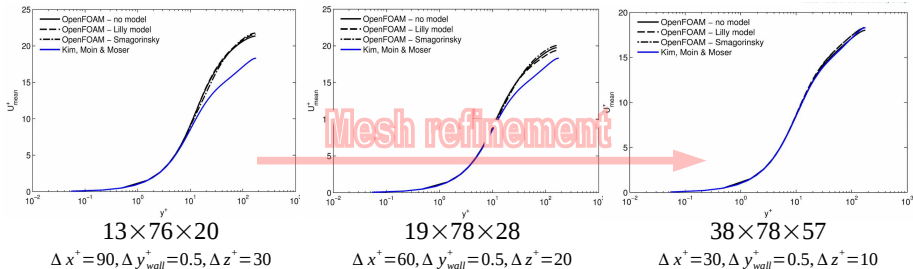


- Are LES results are merit of the SGS model?

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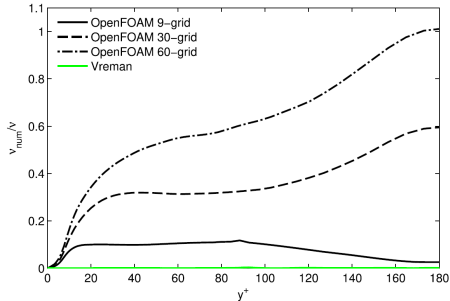
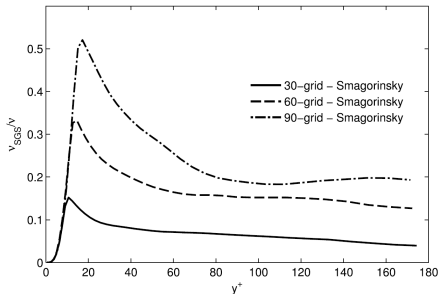


- Are LES results are merit of the SGS model? Apparently **NOT!!!** ✗

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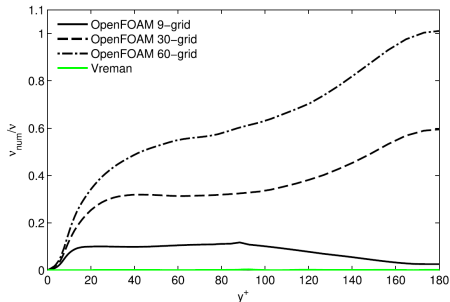
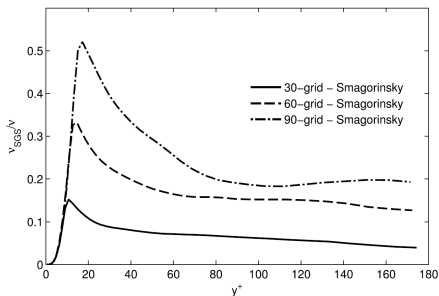


$$\nu_{num} \neq 0$$

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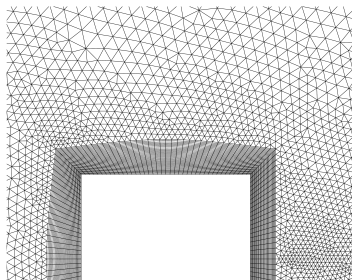
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# Symmetry-preserving discretization

Continuous

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{C}(\mathbf{u}, \mathbf{u}) = \nu \nabla^2 \mathbf{u} - \nabla p$$
$$\nabla \cdot \mathbf{u} = 0$$



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Discrete

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

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$$\mathbf{D} = \mathbf{D}^T \quad \text{def -}$$

# Why collocated arrangements are so popular?

- STAR-CCM+



SIEMENS



- ANSYS-FLUENT



- Code-Saturne



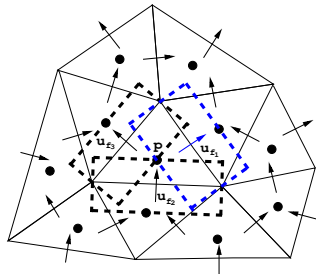
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In staggered meshes

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



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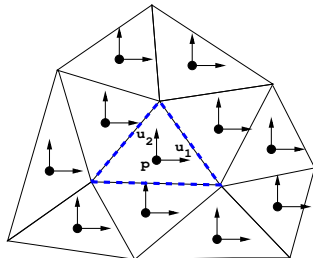
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In collocated meshes

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



# Why collocated arrangements are so popular?

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

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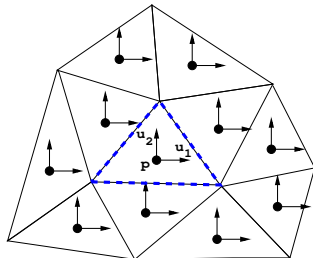
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# Pressure-velocity coupling on collocated grids

A vicious circle that cannot be broken...

In summary<sup>8</sup>:

- Mass:  $M\Gamma_{c \rightarrow s} \mathbf{u}_c = M\Gamma_{c \rightarrow s} \mathbf{u}_c - L_c L_c^{-1} M\Gamma_{c \rightarrow s} \mathbf{u}_c \approx \mathbf{0}_c \quad \mathbf{X}$
- Energy:  $\mathbf{p}_c (L - L_c) \mathbf{p}_c \neq 0 \quad \mathbf{X}$

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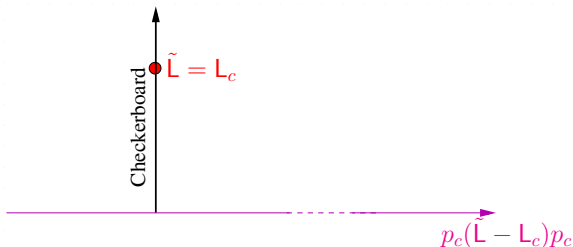
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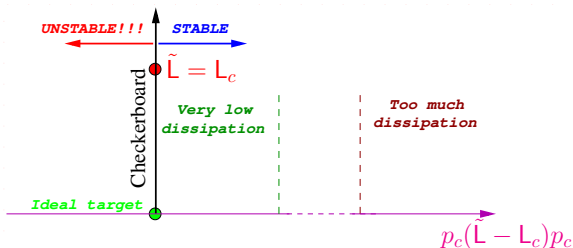
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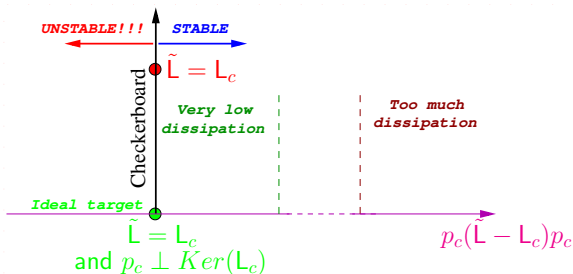
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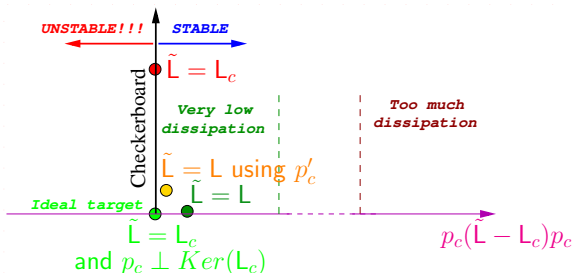
<sup>8</sup>Shashank, J.Larsson, G.laccarino. *A co-located incompressible Navier-Stokes solver with exact mass, momentum and kinetic energy conservation in the inviscid limit*, *Journal of Computational Physics*, 229: 4425-4430,2010.

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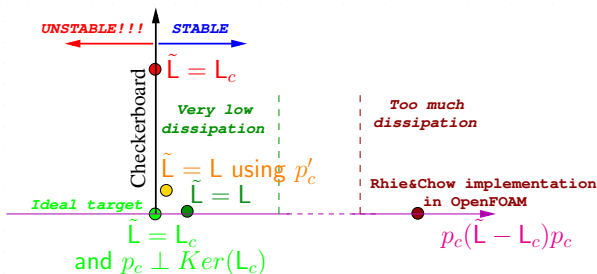
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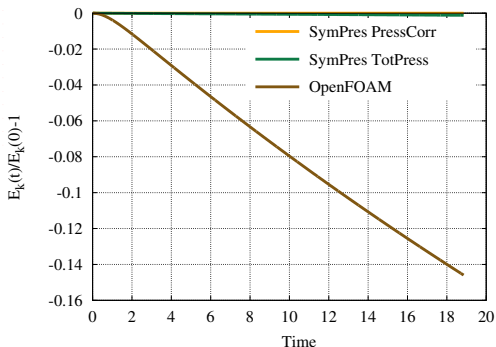
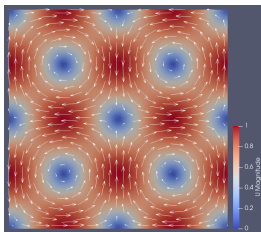
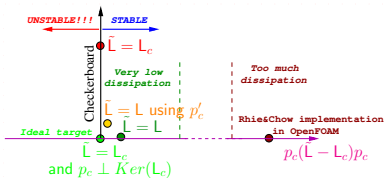
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A vicious circle that ~~cannot be broken~~ can almost be broken...



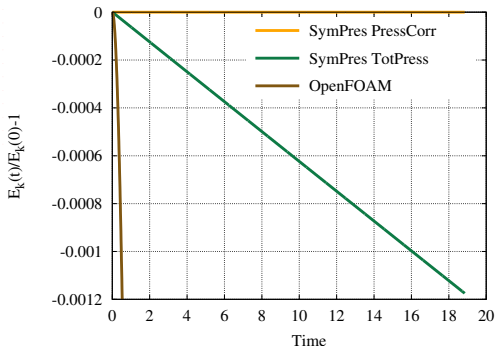
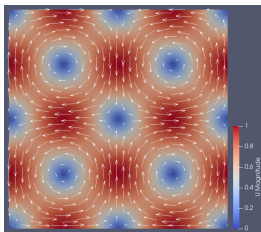
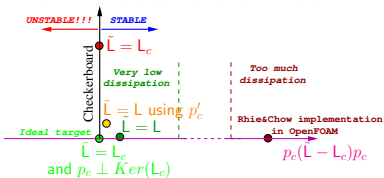
Results for an inviscid Taylor-Green vortex<sup>9</sup>

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# Pressure-velocity coupling on collocated grids

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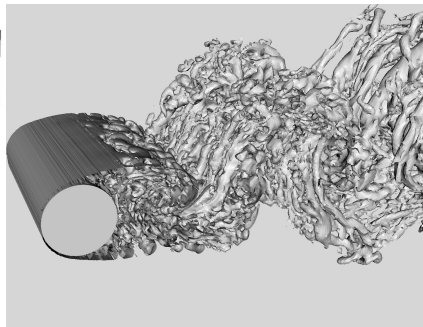
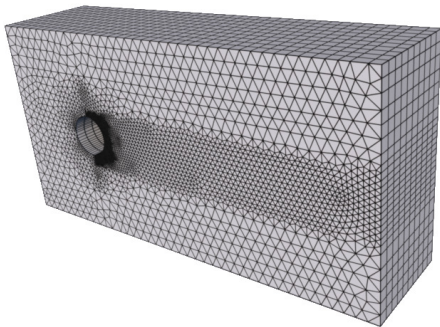
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# Pressure-velocity coupling on collocated grids

## Examples of simulations

Despite these inherent limitations, symmetry-preserving collocated formulation has been successfully used for DNS/LES simulations<sup>10</sup>:

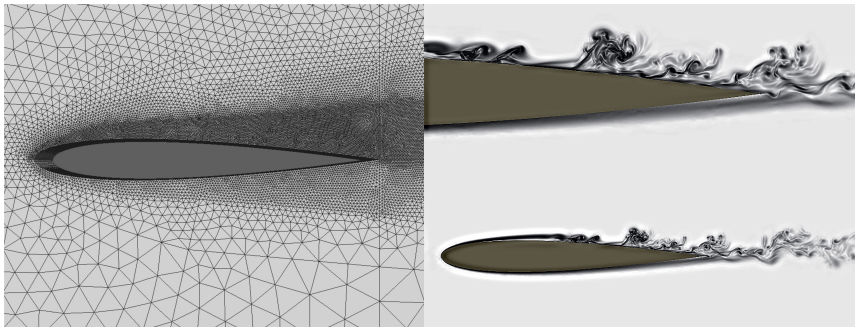


<sup>10</sup>R.Borrell, O.Lehmkuhl, F.X.Trias, A.Oliva. *Parallel Direct Poisson solver for discretizations with one Fourier diagonalizable direction*. **Journal of Computational Physics**, 230:4723-4741, 2011.

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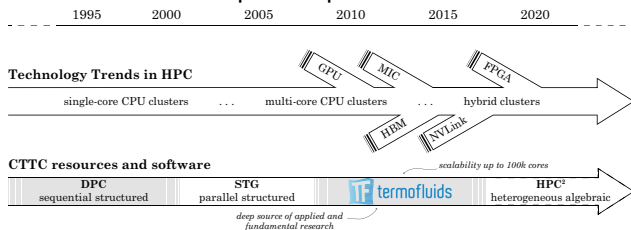


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# Algebra-based approach naturally leads to portability

## Research question #2:

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



**HPC<sup>2</sup>:** 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 presented in this Symposium<sup>11</sup>.

<sup>11</sup>X.Álvarez-Farré, À.Alsaltí-Baldellou, A.Gorobets, A.Oliva, F.X.Trias. *Enabling larger and faster simulations from mesh symmetries. HiFiLeD2 Symposium* Don't miss it!

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

Continuous

Discrete

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

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

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

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

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

$$\langle \nabla^2 \mathbf{a}, \mathbf{b} \rangle = \langle \mathbf{a}, \nabla^2 \mathbf{b} \rangle$$

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

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

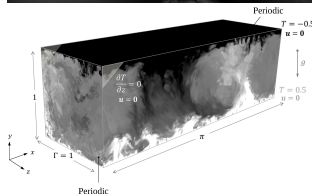
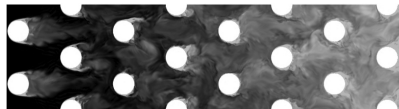
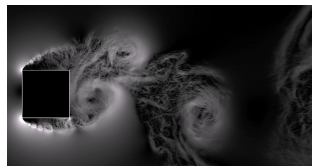
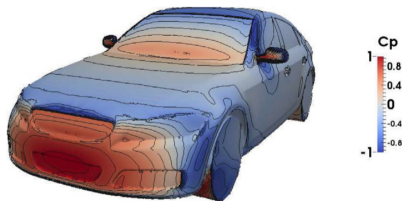
$$\langle \mathbf{a}_h, \mathbf{b}_h \rangle_h = \mathbf{a}_h^T \Omega \mathbf{b}_h$$

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

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

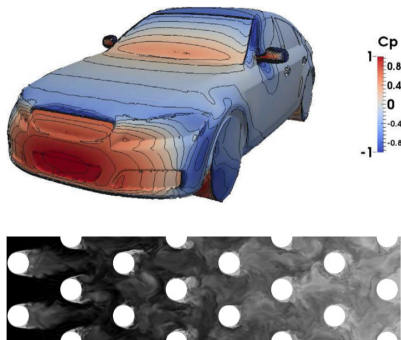
$$\mathbf{D} = \mathbf{D}^T \quad \text{def -}$$

Algebra-based approach naturally leads to portability, to simple and analyzable formulations and opens the door to new strategies<sup>12</sup> to improve its performance...

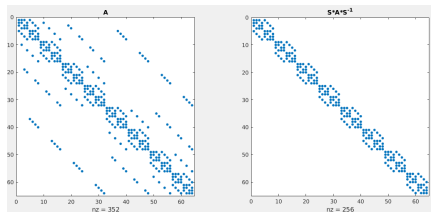


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Algebra-based approach naturally leads to portability, to simple and analyzable formulations and opens the door to new strategies<sup>12</sup> to improve its performance...



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



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

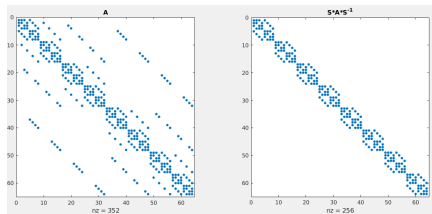
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Benefits for Poisson solver are 3-fold:

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

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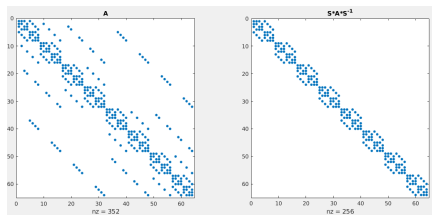
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→ Overall speed-up up to **x2-x3** ✓

→ Memory reduction of  $\approx 2$  ✓

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



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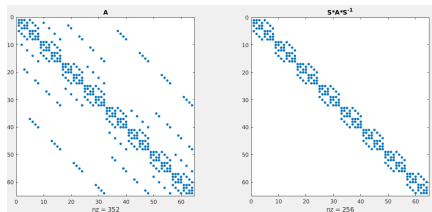
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Other SpMM-based strategies to **increase AI** and **reduce memory footprint**:

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

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

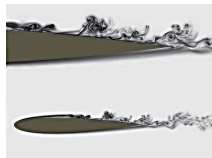


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## Concluding remarks

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

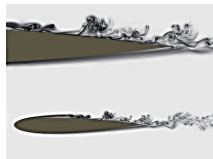


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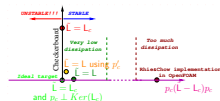
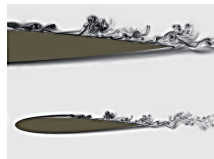
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On-going research:

- **Rethinking** standard CFD operations (e.g. flux limiters<sup>13</sup>, CFL,...) to adapt them into an algebraic framework (Motivation: maintaining a minimal number of basic kernels is crucial for portability!!!)
- Symmetry-preserving formulations for **staggered unstructured** grids.

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Thank you for your virtual  
attendance