



Centre Tecnològic de Transferència de Calor  
UNIVERSITAT POLITÈCNICA DE CATALUNYA



## Robust and reliable DNS and LES on unstructured grids

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

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# Robust and reliable DNS and LES on unstructured grids: playing with matrices to preserve symmetries using a small set of algebraic kernels

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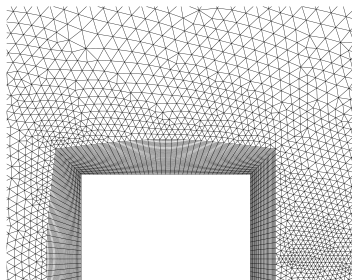
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- 2 Preserving symmetries at discrete level
- 3 Portability and beyond
- 4 Rethinking CFD
- 5 Conclusions

# 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  $Re = 22000$

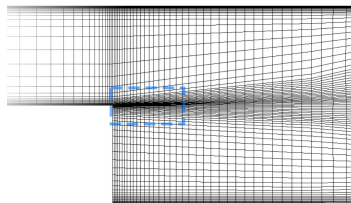
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<sup>1</sup>F.X.Trias, A.Gorobets, A.Oliva. *Turbulent flow around a square cylinder at Reynolds number 22000: a DNS study*, **Computers&Fluids**, 123:87-98, 2015.

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

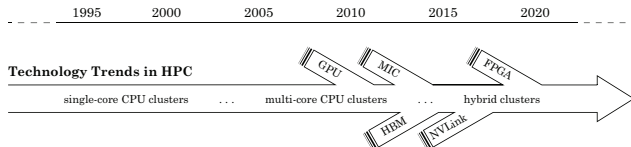
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<sup>2</sup>A.Pont-Vílchez, F.X.Trias, A.Gorobets, A.Oliva. *DNS of Backward-Facing Step flow at  $Re_\tau = 395$  and expansion ratio 2*. **Journal of Fluid Mechanics**, 863:341-363, 2019.

# 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. *A hierarchical parallel implementation for heterogeneous computing. Application to algebra-based CFD simulations on hybrid supercomputers.* **Computers & Fluids**, 214:104768, 2021.

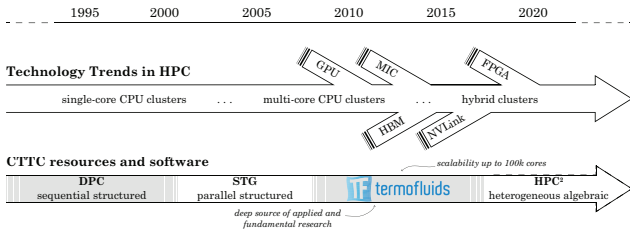
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# Motivation

## 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<sup>3,4</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 conference<sup>5</sup>.

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# Motivation

Frequently used general purpose CFD codes:

- STAR-CCM+



**SIEMENS**



- ANSYS-FLUENT



- Code-Saturne



- OpenFOAM





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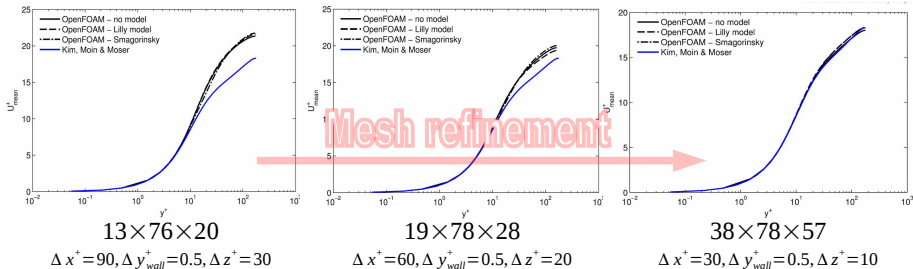


Main common characteristics of LES in such codes:

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

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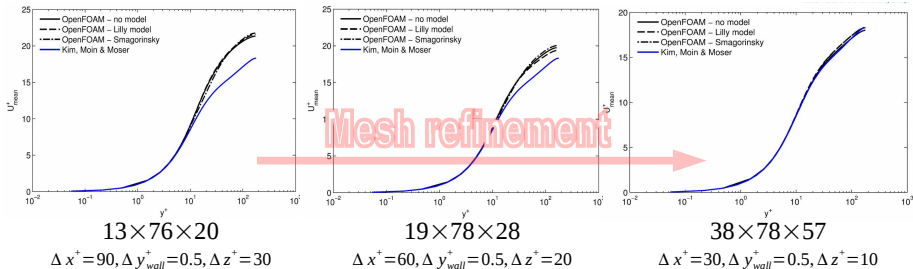
OpenFOAM® LES<sup>6</sup> results of a turbulent channel for at  $Re_\tau = 180$



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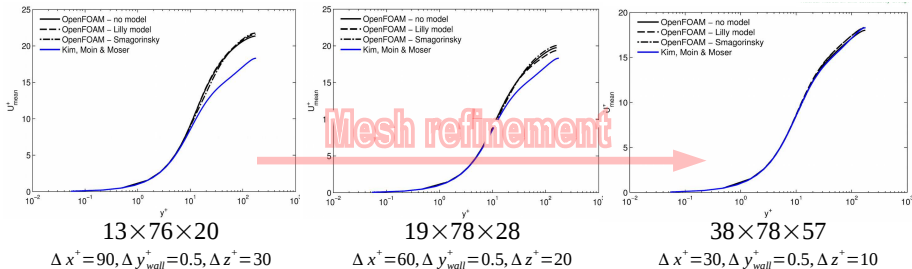


- Are LES results are merit of the SGS model?

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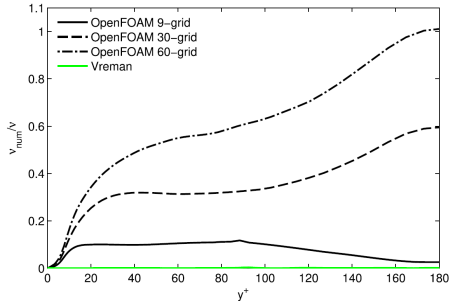
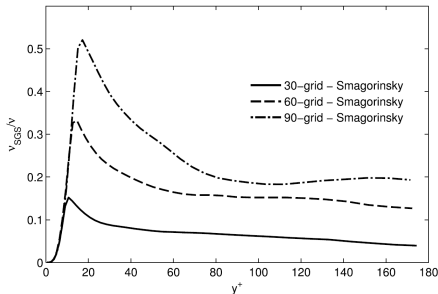


- Are LES results are merit of the SGS model? Apparently **NOT!!!** ✘

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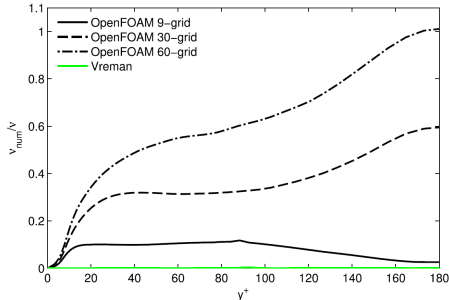
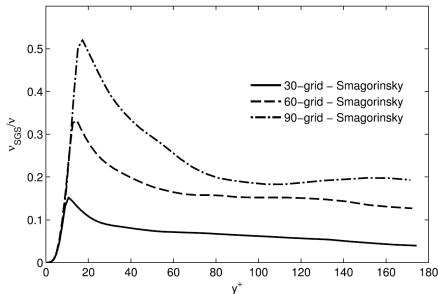


$$\nu_{num} \neq 0$$

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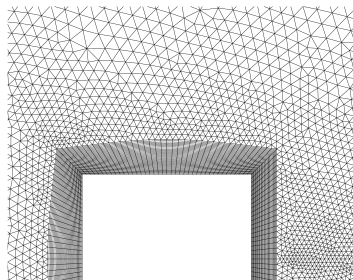
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# Symmetry-preserving discretization

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

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

# Why collocated arrangements are so popular?

- STAR-CCM+



- ANSYS-FLUENT



- Code-Saturne



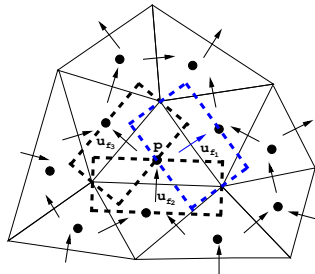
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In staggered meshes

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



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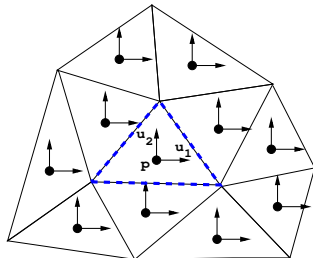
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In collocated meshes

- $p$ - $\mathbf{u}_c$  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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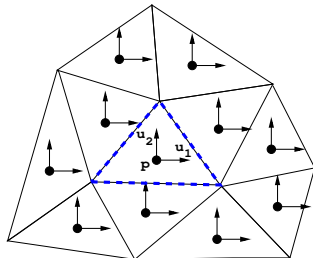
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# Pressure-velocity coupling on collocated grids

A vicious circle that cannot be broken...

In summary<sup>8</sup>:

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

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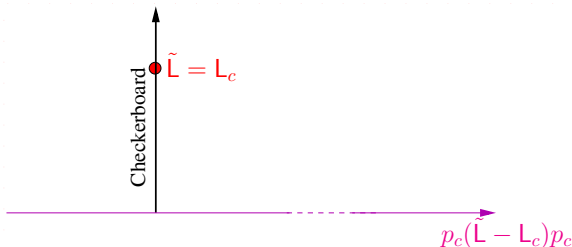
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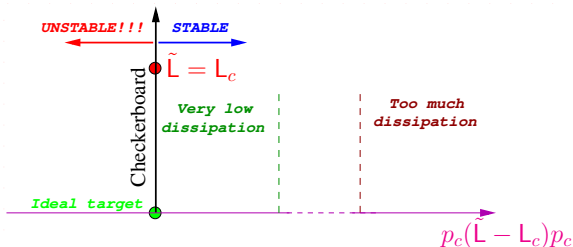
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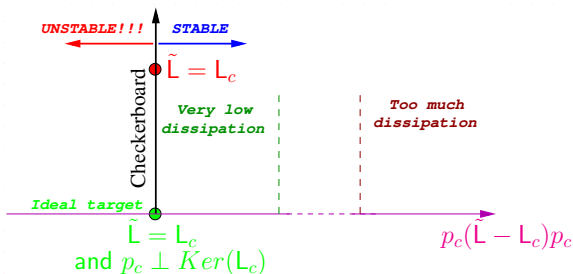
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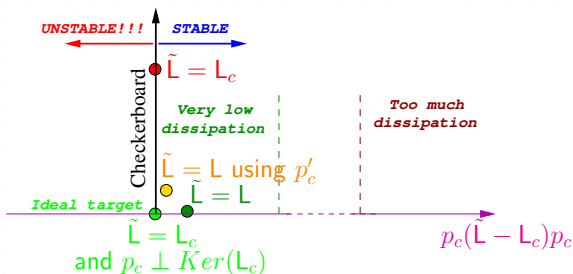
<sup>8</sup>Shashank, J.Larsson, G.laccarino. *A co-located incompressible Navier-Stokes solver with exact mass, momentum and kinetic energy conservation in the inviscid limit*, *Journal of Computational Physics*, 229: 4425-4430,2010.

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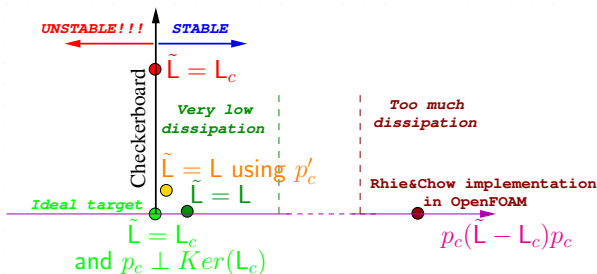
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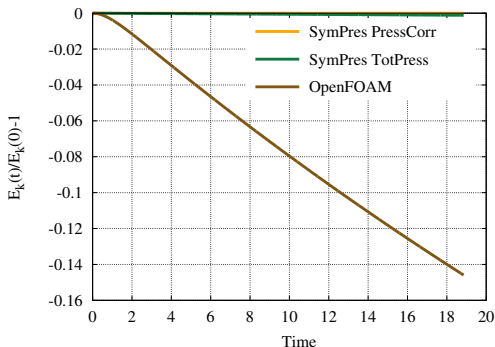
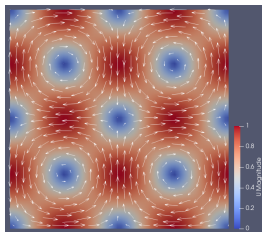
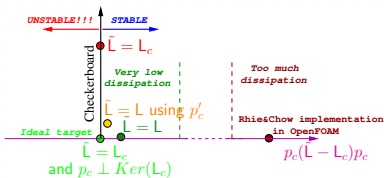
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A vicious circle that ~~cannot be broken~~ can almost be broken...



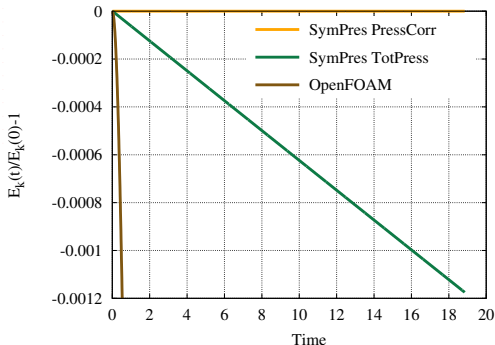
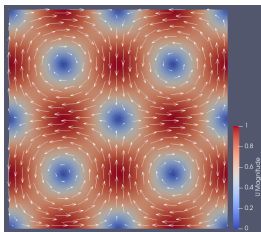
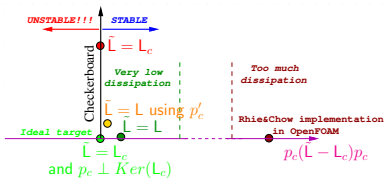
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# Pressure-velocity coupling on collocated grids

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



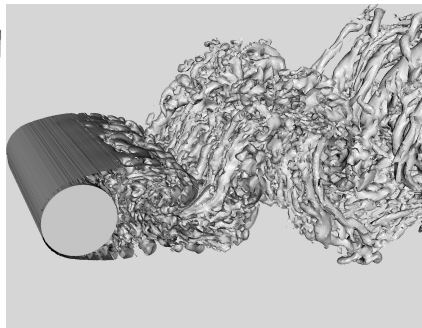
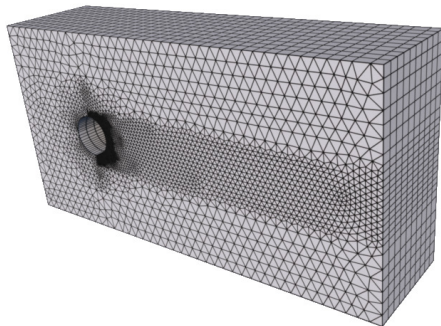
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# Pressure-velocity coupling on collocated grids

## Examples of simulations

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

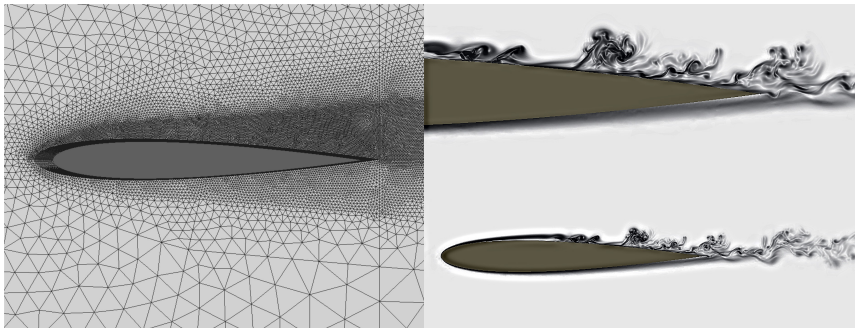


<sup>10</sup>R.Borrell, O.Lehmkuhl, F.X.Trias, A.Oliva. *Parallel Direct Poisson solver for discretizations with one Fourier diagonalizable direction*. **Journal of Computational Physics**, 230:4723-4741, 2011.

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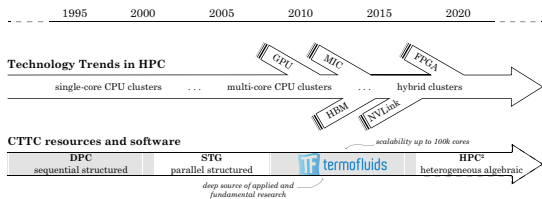


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# Algebra-based approach naturally leads to portability

## 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/were presented in this conference<sup>11</sup>.

<sup>11</sup> A. Alsalti-Baldellou, G. Colomer, J.A. Hopman, X. Álvarez-Farré, A. Gorobets, F.X. Trias, A. Oliva. *Reliable overnight industrial LES: challenges and limitations. Application to CSP technologies. On Friday at 15:40*

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

Continuous

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

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

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

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

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

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

Discrete

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

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

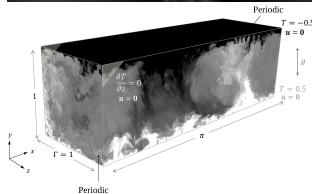
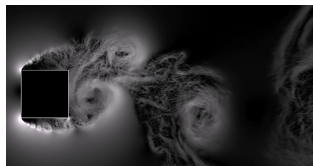
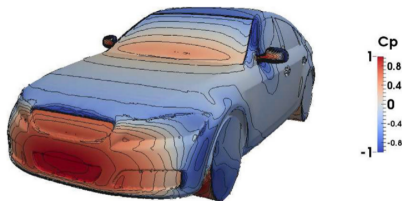
$$\langle \mathbf{a}_h, \mathbf{b}_h \rangle_h = \mathbf{a}_h^T \Omega \mathbf{b}_h$$

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

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

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

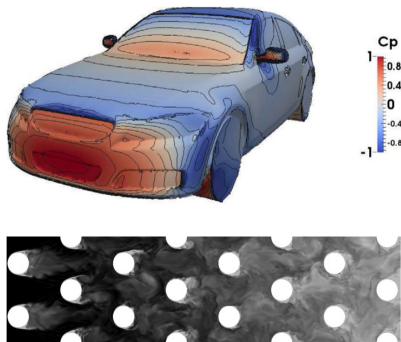
Algebra-based approach naturally leads to portability, to simple and analyzable formulations and opens the door to new strategies<sup>12,13</sup> to improve its performance...



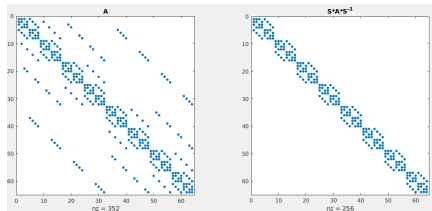
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$$\hat{\mathbf{L}} = \mathbf{S}\mathbf{L}\mathbf{S}^{-1} = \mathbf{I} \otimes \mathbf{L}_{inn} + \text{diag}(\mathbf{d})$$



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

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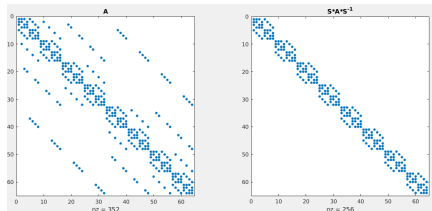
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Benefits for Poisson solver are 3-fold:

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

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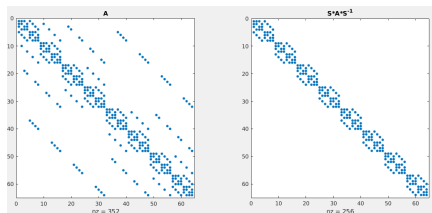
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- Reduction of memory footprint
- Reduction in the number of iterations

→ Overall speed-up up to **x2-x3** ✓

→ Memory reduction of  $\approx 2$  ✓

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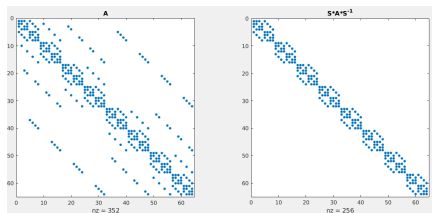
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Algebra-based approach naturally leads to portability, to simple and analyzable formulations and opens the door to new strategies<sup>12,13</sup> to improve its performance...

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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# Rethinking standard CFD operations

In summary...

**Leitmotiv**: relying on a **minimal set of (algebraic) kernels** is crucial for code **portability** and **maintenance!!!**

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- Computational challenge: SpMV has a low AI
  - Solution: make use of SpMM whenever possible (multiple transport equations, spatial symmetries, parallel-in-time simulations, parametric studies,...) to increase AI and, therefore, performance.
  - Positive side-effects: reduction of memory footprint (crucial for GPUs), improvement of the convergence for the Poisson solver...

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- Implementation challenge: there still exists a list of standard CFD methods that do not seem to fit well on an algebraic framework (e.g. flux limiters<sup>14</sup>, boundary conditions, CFL condition,...).
  - Dilemma: "add more and more specific kernels" vs "rethink them"

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# Rethinking standard CFD operations

CFL-like condition

**Step #1:** forget about classical formulae from textbooks...

$$\cancel{\Delta t \leq C_{conv} \left( \frac{\Delta x}{U} \right)_{\min}} \quad \text{and} \quad \cancel{\Delta t \leq C_{diff} \left( \frac{\Delta x^2}{\nu} \right)_{\min}}$$

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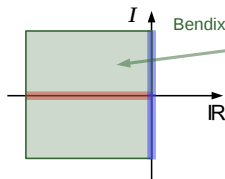
...and replace it by an eigenbouding problem of  $\mathbf{C}(\mathbf{u}_s)$  and  $\mathbf{D}$  matrices

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

$$\mathbf{C}(\mathbf{u}_s) \mathbf{v} = \lambda \mathbf{v}$$

$$\mathbf{D} \mathbf{v} = \lambda \mathbf{v}$$

$$(-\mathbf{C}(\mathbf{u}_s) + \mathbf{D}) \mathbf{v} = \lambda \mathbf{v}$$



Bendixson (1900)

SUR LES RACINES D'UNE ÉQUATION FONDAMENTALE:

PAR  
IVAR BENDIXSON  
À STOCKHOLM.

Dans diverses recherches d'analyse on est conduit à l'étude de l'équation suivante:

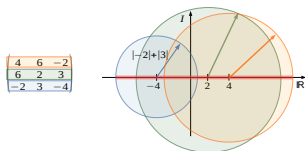
$$\lambda^{n-1} + a_{n-1} \lambda^{n-2} + \dots + a_1 \lambda + a_0 = 0$$



# Rethinking standard CFD operations

## CFL-like condition

**Step #2:** compute eigenbounds of  $C(u_s)$  and  $D$  in an inexpensive way<sup>15</sup>



$$\rho(D) \leq \rho^{\text{Gersh}}(D)$$

$$\rho(C) \leq \rho^{\text{Gersh}}(C)$$

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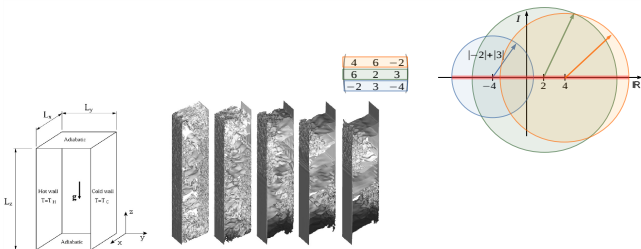
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$$\rho(\mathbf{D}) \leq \rho^{\text{Gersh}}(\mathbf{D})$$

$$\rho(\mathbf{C}) \leq \rho^{\text{Gersh}}(\mathbf{C})$$



**Table 1.** Tests for the air-filled ( $Pr=0.71$ ) differentially heated cavity at Rayleigh number  $Ra=3 \times 10^{10}$  and height aspect ratio 4; averaged results correspond to the statistically steady state

	$N_x$	$N_y$	$N_z$	$\phi/(\pi/2)$	$\bar{\delta}t_{\text{CFL+AB2}}$	$\bar{\delta}t_{\text{EigenCD+k1L2}}$	$\bar{\delta}t_{\text{EigenCD+k1L2}}/\bar{\delta}t_{\text{CFL+AB2}}$
MeshA	128	338	778	0.072	$1.04 \times 10^{-4}$	$3.02 \times 10^{-4}$	2.90
MeshB	64	168	338	0.158	$4.31 \times 10^{-4}$	$1.21 \times 10^{-3}$	2.80
MeshC	32	84	168	0.252	$1.80 \times 10^{-3}$	$4.69 \times 10^{-3}$	2.59
MeshD	32	56	112	0.408	$4.21 \times 10^{-3}$	$8.75 \times 10^{-3}$	2.08
MeshE	16	42	84	0.504	$6.88 \times 10^{-3}$	$1.35 \times 10^{-2}$	1.96

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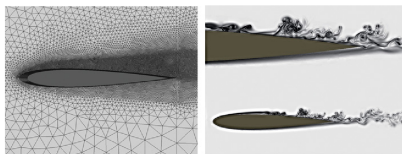
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CFL-like condition

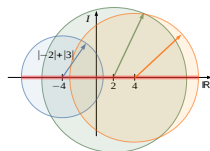
**Step #2:** compute eigenbounds of  $C(u_s)$  and  $D$  in an inexpensive way<sup>15</sup>

$$\rho(D) \leq \rho^{\text{Gersh}}(D)$$

$$\rho(C) \leq \rho^{\text{Gersh}}(C)$$



4	6	-2
6	2	3
-2	3	-4



**Table 2.** Tests for the flow around a NACA 0012 airfoil at Reynolds number  $5 \times 10^4$  and an angle of attack of  $5^\circ$ ; averaged results correspond to the statistically steady state

	$N_x$	Mesh2D	$\varphi/(\pi/2)$	$\bar{\delta}_t^{\text{CFL+AB2}}$	$\bar{\delta}_t^{\text{EigenCD}+\kappa\text{IL2}}$	$\bar{\delta}_t^{\text{EigenCD}+\kappa\text{IL2}}/\bar{\delta}_t^{\text{CFL+AB2}}$
UMeshA	64	$\approx 2.65 \times 10^5$	0.593	$4.69 \times 10^{-5}$	$1.30 \times 10^{-4}$	2.77
UMeshB	32	$\approx 4.69 \times 10^4$	0.956	$1.61 \times 10^{-4}$	$6.86 \times 10^{-4}$	4.27

<sup>15</sup>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.

# Rethinking standard CFD operations

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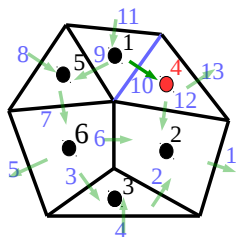
## Step #3:

reformulate the problem in a way that we avoid constructing  $C(\mathbf{u}_s)$  and  $D$

$$C(\mathbf{u}_s) \equiv -1/2 T_{CS}^T A_s U_s |T_{CS}| \quad D \equiv -T_{CS}^T A_s \Lambda_s \Delta_s^{-1} T_{CS}$$

$$T_{sc} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{matrix} 10 \\ 12 \\ 13 \end{matrix}$$

face-to-cell oriented incidence matrix



# Rethinking standard CFD operations

CFL-like condition

**Step #3 ... #4 (some maths that would take too long to explain):**  
reformulate the problem in a way that we avoid constructing  $\mathbf{C}(\mathbf{u}_s)$  and  $\mathbf{D}$

$$\mathbf{C}(\mathbf{u}_s) \equiv -1/2 \mathbf{T}_{cs}^T \mathbf{A}_s \mathbf{U}_s |\mathbf{T}_{cs}| \quad \mathbf{D} \equiv -\mathbf{T}_{cs}^T \mathbf{A}_s \Lambda_s \Delta_s^{-1} \mathbf{T}_{cs}$$

$$\rho(\mathbf{D}) \leq \rho^{\text{Gersh}}(\mathbf{D})$$

$$\rho(\mathbf{C}) \leq \rho^{\text{Gersh}}(\mathbf{C})$$

where  $\mathbf{T}_{cs}$  is the face-to-cell oriented incidence matrix;  $\tilde{\Delta}_s \equiv \mathbf{A}_s \Lambda_s \Delta_s^{-1}$  (diffusivity-like fluxes) and  $\tilde{\mathbf{F}}_s \equiv \mathbf{A}_s \mathbf{U}_s$  (mass fluxes) are diagonal matrices.

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CFL-like condition

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$$\mathbf{C}(\mathbf{u}_s) \equiv -1/2 \mathbf{T}_{cs}^T \mathbf{A}_s \mathbf{U}_s |\mathbf{T}_{cs}| \quad \mathbf{D} \equiv -\mathbf{T}_{cs}^T \mathbf{A}_s \Lambda_s \Delta_s^{-1} \mathbf{T}_{cs}$$

$$\rho(\mathbf{D}) \leq \dots \leq \rho(\mathbf{T}_{cs} \mathbf{T}_{cs}^T \tilde{\Delta}_s) \leq \max_{\text{SpMV}} \left( \overbrace{|\mathbf{T}_{cs} \mathbf{T}_{cs}^T| \text{diag}(\tilde{\Delta}_s)}^{\text{Constant matrix}} \right)$$

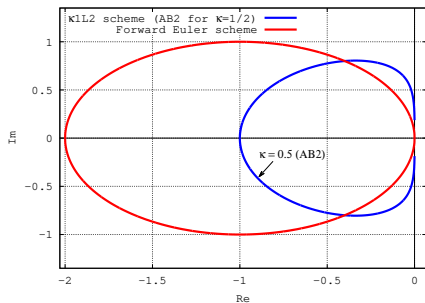
$$\rho(\mathbf{C}) \leq \dots \leq 1/4 \rho(|\mathbf{T}_{cs} \mathbf{T}_{cs}^T| |\tilde{\mathbf{F}}_s|) \leq 1/4 \max_{\text{SpMV}} \left( \overbrace{|\mathbf{T}_{cs} \mathbf{T}_{cs}^T| \text{diag}(|\tilde{\mathbf{F}}_s|)}^{\text{Constant matrix}} \right)$$

where  $\mathbf{T}_{cs}$  is the face-to-cell oriented incidence matrix;  $\tilde{\Delta}_s \equiv \mathbf{A}_s \Lambda_s \Delta_s^{-1}$  (diffusivity-like fluxes) and  $\tilde{\mathbf{F}}_s \equiv \mathbf{A}_s \mathbf{U}_s$  (mass fluxes) are diagonal matrices.

# Rethinking standard CFD operations

CFL-like condition

**Step #5:** self-adaptation of the stability region

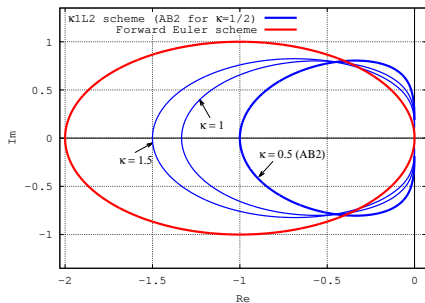


$$\frac{\left(\kappa + \frac{1}{2}\right) \phi^{n+1} - 2\kappa\phi^n + \left(\kappa - \frac{1}{2}\right) \phi^{n-1}}{\Delta t} = f \left( (1 + \kappa)\phi^n - \kappa\phi^{n-1} \right)$$

# Rethinking standard CFD operations

## CFL-like condition

### Step #5: self-adaptation of the stability region



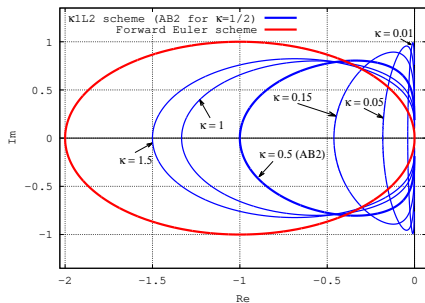
$$\frac{\left(\kappa + \frac{1}{2}\right) \phi^{n+1} - 2\kappa\phi^n + \left(\kappa - \frac{1}{2}\right) \phi^{n-1}}{\Delta t} = f \left( (1 + \kappa)\phi^n - \kappa\phi^{n-1} \right)$$



# Rethinking standard CFD operations

## CFL-like condition

### Step #5: self-adaptation of the stability region

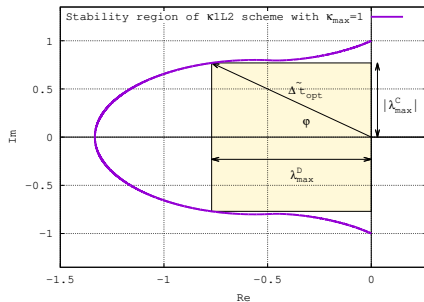
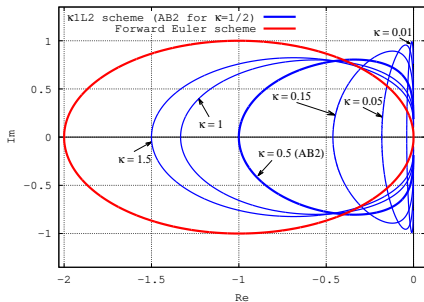


$$\frac{(\kappa + \frac{1}{2}) \phi^{n+1} - 2\kappa\phi^n + (\kappa - \frac{1}{2}) \phi^{n-1}}{\Delta t} = f((1 + \kappa)\phi^n - \kappa\phi^{n-1})$$

# Rethinking standard CFD operations

## CFL-like condition

### Step #5: self-adaptation of the stability region

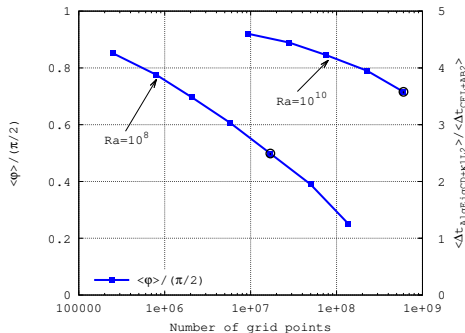


$$\frac{\left(\kappa + \frac{1}{2}\right) \phi^{n+1} - 2\kappa\phi^n + \left(\kappa - \frac{1}{2}\right) \phi^{n-1}}{\Delta t} = f\left(\left(1 + \kappa\right)\phi^n - \kappa\phi^{n-1}\right)$$

# Rethinking standard CFD operations

CFL-like condition: results

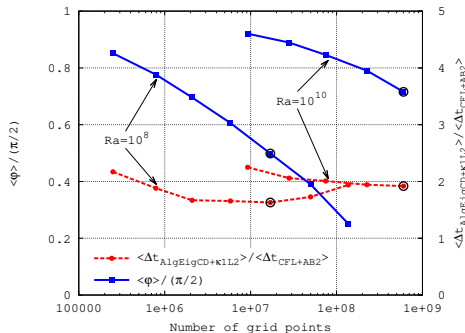
## Numerical test #1: air-filled Rayleigh–Bénard convection



# Rethinking standard CFD operations

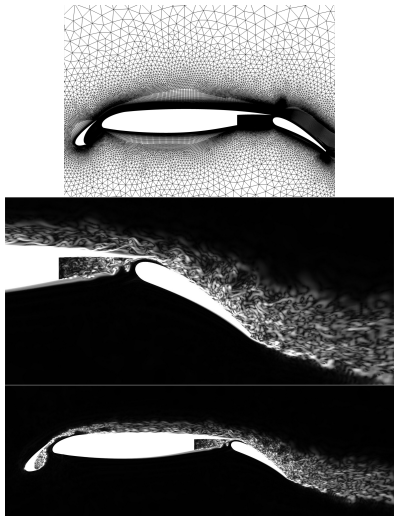
CFL-like condition: results

## Numerical test #1: air-filled Rayleigh–Bénard convection

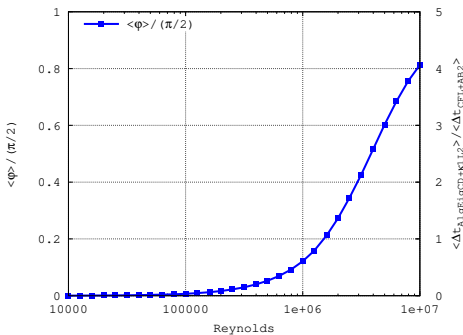


# Rethinking standard CFD operations

CFL-like condition: results

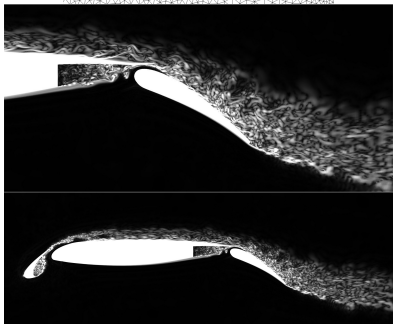
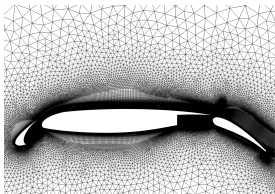


## Numerical test #2: 30P30N airfoil

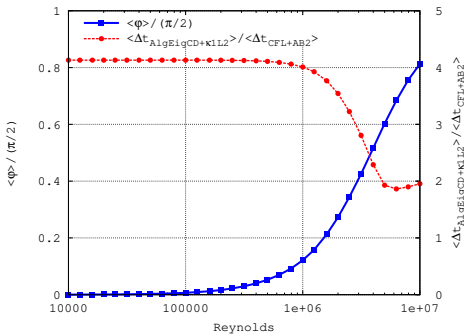


# Rethinking standard CFD operations

CFL-like condition: results

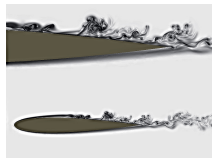


## Numerical test #2: 30P30N airfoil



## Concluding remarks

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



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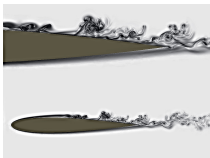
<sup>16</sup>N.Valle, X.Álvarez, A.Gorobets, J.Castro, A.Oliva, F.X.Trias. *On the implementation of flux limiters in algebraic frameworks*. **Computer Physics Communications**, 271:108230, 2022.





## Concluding remarks

- **Preserving symmetries** either using staggered or collocated formulations is the key point for **reliable LES/DNS** simulations.
- Algebra-based approach naturally leads to **portability**, to simple and **analyzable** formulations and opens the door to **new strategies to improve its performance**.



On-going research:

- **Rethinking** standard CFD operations (e.g. flux limiters<sup>16</sup>, boundary conditions, **CFL**,...) to adapt them into an algebraic framework (Motivation: maintaining a minimal number of basic kernels is crucial for portability!!!)

<sup>16</sup>N.Valle, X.Álvarez, A.Gorobets, J.Castro, A.Oliva, F.X.Trias. *On the implementation of flux limiters in algebraic frameworks*. **Computer Physics Communications**, 271:108230, 2022.

# Thank you for your attendance