



Centre Tecnològic de Transferència de Calor  
UNIVERSITAT POLITÈCNICA DE CATALUNYA



# Paving the way for DNS and LES on unstructured grids

F.Xavier Trias<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

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# Paving the (right?) way for DNS and LES on unstructured grids: fully conservative collocated/staggered discretizations

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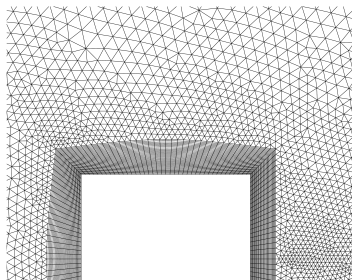
# Contents

- 1 Motivation
- 2 Preserving symmetries: collocated vs staggered
- 3 Building a staggered formulation
- 4 Portability and beyond
- 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  $Re = 22000$

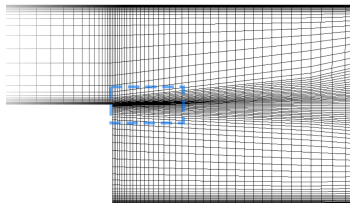
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<sup>1</sup>F.X.Trias, A.Gorobets, A.Oliva. *Turbulent flow around a square cylinder at Reynolds number 22000: a DNS study*, **Computers&Fluids**, 123:87-98, 2015.

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

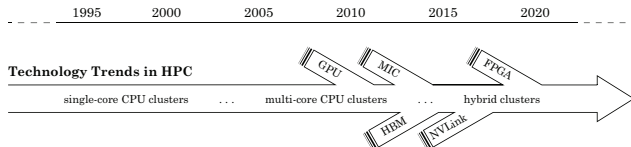
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<sup>2</sup>A.Pont-Vílchez, F.X.Trias, A.Gorobets, A.Oliva. *DNS of Backward-Facing Step flow at  $Re_\tau = 395$  and expansion ratio 2*. **Journal of Fluid Mechanics**, 863:341-363, 2019.

# 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, G.Oyarzun. *HPC<sup>2</sup> - a fully portable algebra-dominant framework for heterogeneous computing. Application to CFD*. **Computers & Fluids**, 173:285-292, 2018.

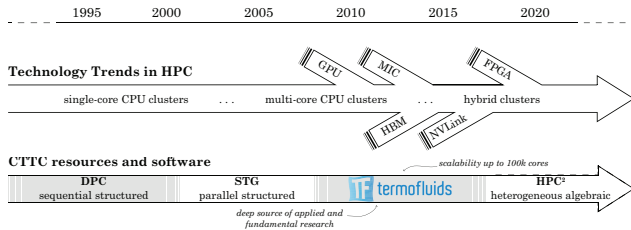
<sup>4</sup>X.Álvarez, A.Gorobets, F.X.Trias. *A hierarchical parallel implementation for heterogeneous computing. Application to algebra-based CFD simulations on hybrid supercomputers*. **Computers & Fluids**, 214:104768, 2021.

<sup>5</sup>X.Álvarez, A.Gorobets, F.X.Trias, A.Oliva. *NUMA-aware strategies for the efficient execution of CFD simulations on CPU supercomputers* **ParCFD2021**. Don't miss it!

# 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<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. NUMA-aware execution strategies for CFD are presented in this conference<sup>5</sup>.

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

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# Motivation

Frequently used general purpose CFD codes:

- STAR-CCM+



**SIEMENS**



- ANSYS-FLUENT



- Code-Saturne



- OpenFOAM

Open  FOAM®



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Frequently used general purpose CFD codes:

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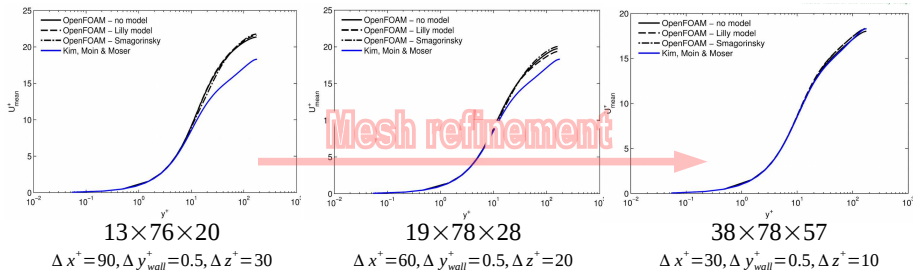
Main common characteristics of LES in such codes:

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



# Motivation

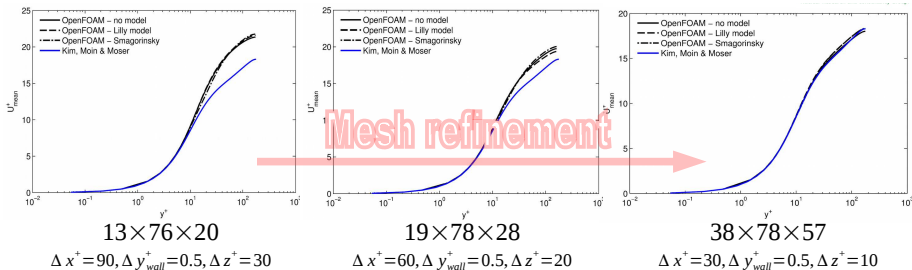
OpenFOAM® LES<sup>6</sup> results of a turbulent channel for at  $Re_\tau = 180$



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

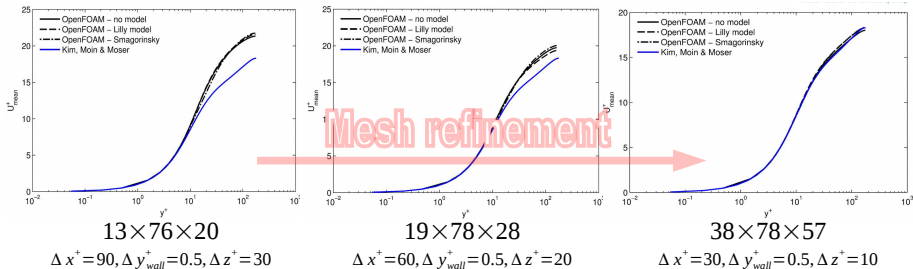


- Are LES results are merit of the SGS model?

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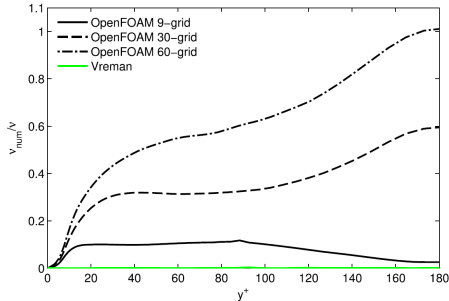
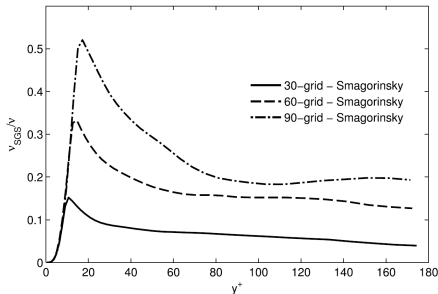


- Are LES results are merit of the SGS model? Apparently **NOT!!!** ✘

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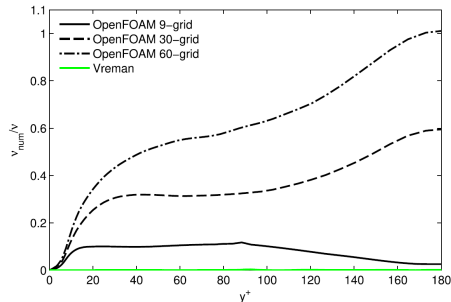
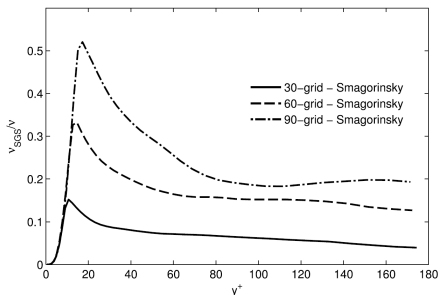


$$v_{num} \neq 0$$

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

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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

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

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

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

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

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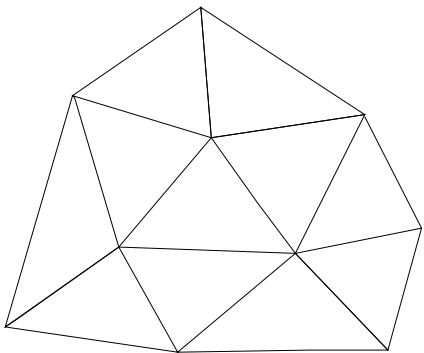
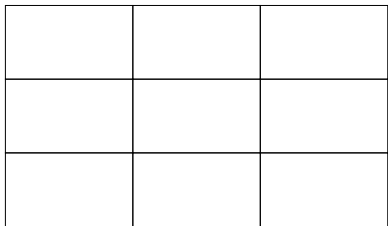
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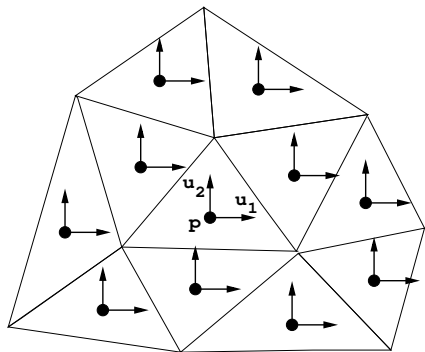
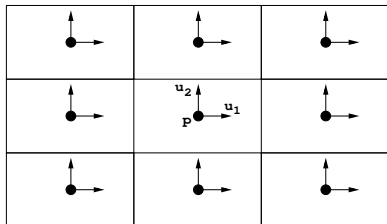
$$\mathbf{D} = \mathbf{D}^T \quad \text{def -}$$

# Collocated vs staggered



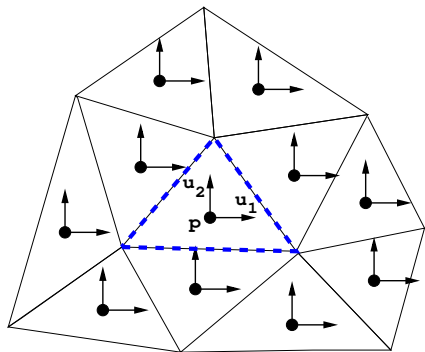
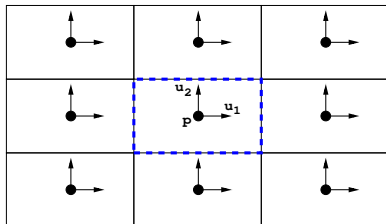
# Collocated vs staggered

*Collocated*

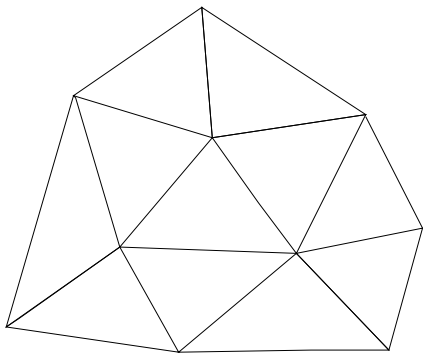
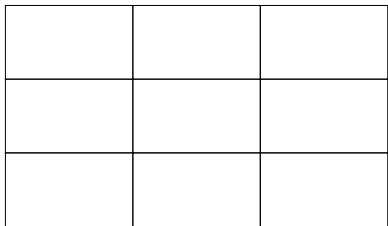


# Collocated vs staggered

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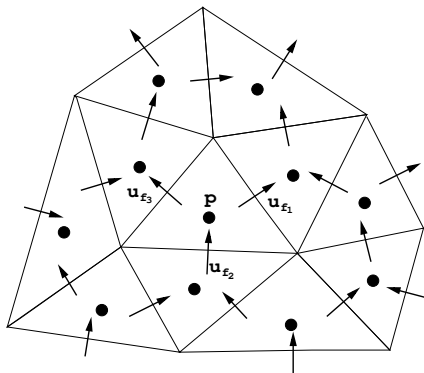
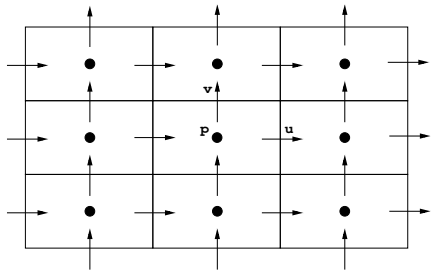


# Collocated vs staggered



# Collocated vs staggered

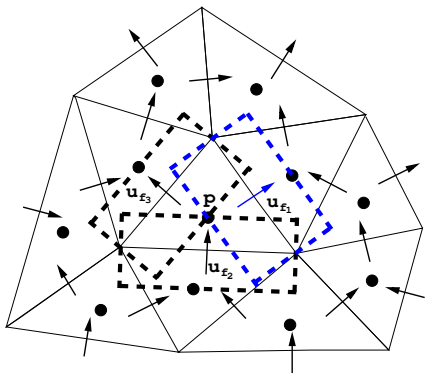
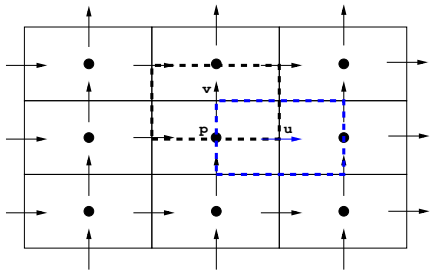
*Staggered*





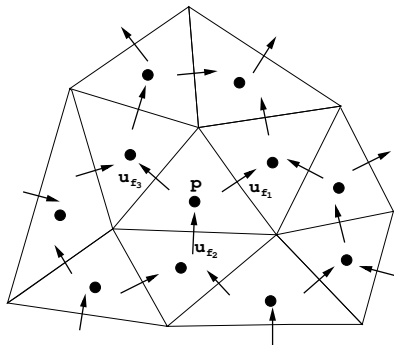
# Collocated vs staggered

*Staggered*



# Why staggered?

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

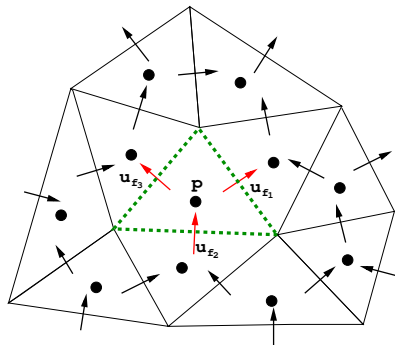


# Why staggered?

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Let's consider we have  $\mathbf{u}_s$  such as

$$\mathbf{M}\mathbf{u}_s \neq \mathbf{0}_c$$



# Why staggered?

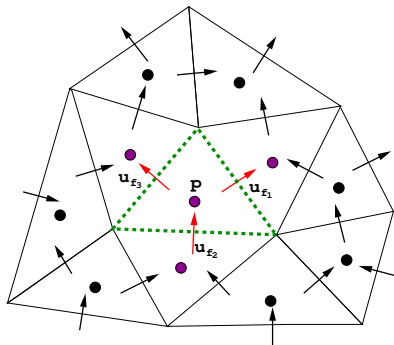
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then, we can easily project  $\mathbf{u}_s$

$$\mathbf{u}_s = \mathbf{u}_s - \mathbf{G}\mathbf{p}_c$$



# Why staggered?

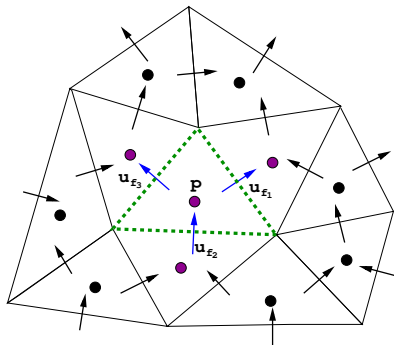
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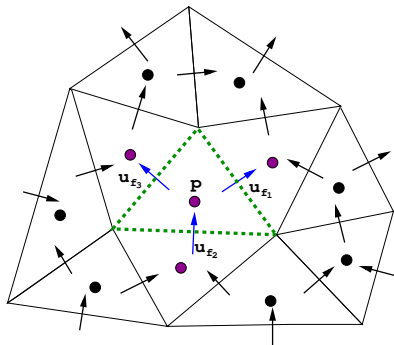
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Finally, this leads to a Poisson eq.

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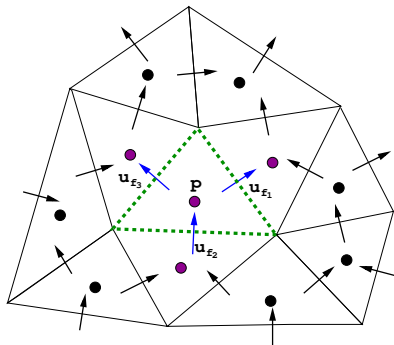
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$$\mathbf{M}\mathbf{G}\mathbf{p}_c = \mathbf{M}\mathbf{u}_s$$

$$\text{If } \Omega_s \mathbf{G} = -\mathbf{M}^T$$

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



# Why staggered? Everything seems to be in the right place!

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

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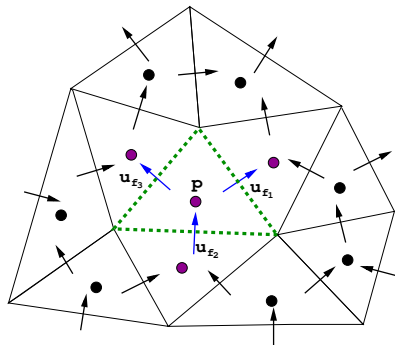
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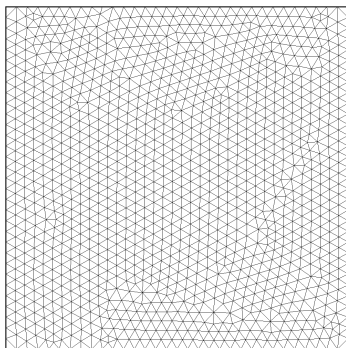
$$\text{If } \Omega_s \mathbf{G} = -\mathbf{M}^T \implies \langle \mathbf{u}_s, \mathbf{G}\mathbf{p}_c \rangle_h = \mathbf{u}_s^T \Omega_s \mathbf{G}\mathbf{p}_c = -(\mathbf{M}\mathbf{u}_s)^T \mathbf{p}_c = 0$$

$$\langle \nabla \cdot \mathbf{a}, \varphi \rangle = -\langle \mathbf{a}, \nabla \varphi \rangle \implies \langle \mathbf{u}, \nabla p \rangle = -\langle \nabla \cdot \mathbf{u}, p \rangle = 0$$

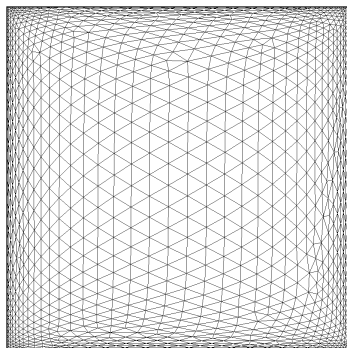


# But is this discrete Laplacian accurate?

Without stretching



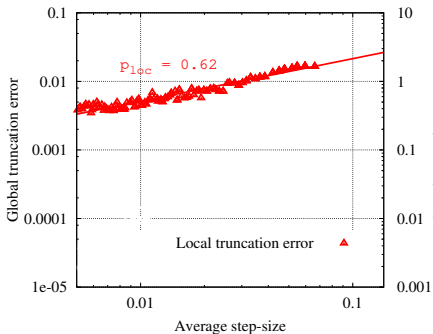
With stretching



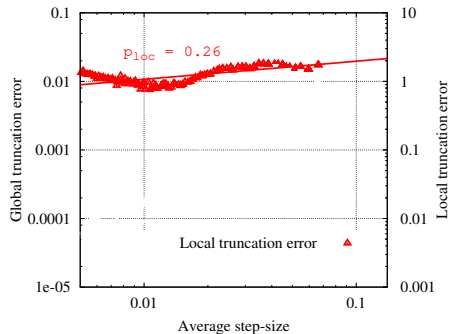
$$\nabla^2 \varphi = f(x, y) \quad \text{with } f(x, y) = \nabla^2(k^{-2} \sin(kx) \sin(ky)) \text{ and } k = 25\pi$$

# But is this discrete Laplacian accurate?

## Without stretching



## With stretching

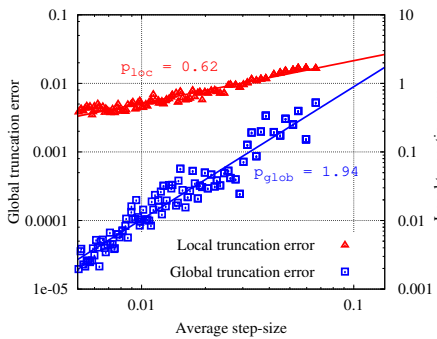


$$\nabla^2 \varphi = f(x, y) \quad \text{with } f(x, y) = \nabla^2 (k^{-2} \sin(kx) \sin(ky)) \text{ and } k = 25\pi$$

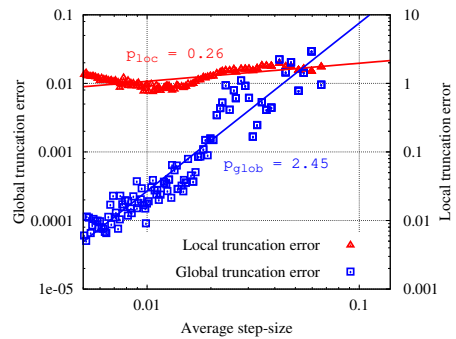
# But is this discrete Laplacian accurate?

Yes, even for distorted unstructured meshes! And symmetries are preserved!

Without stretching












With stretching



$$\nabla^2 \varphi = f(x, y) \quad \text{with } f(x, y) = \nabla^2(k^{-2} \sin(kx) \sin(ky)) \text{ and } k = 25\pi$$

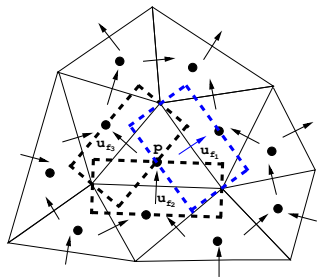
# Then, why collocated arrangements are so popular?

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

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

In staggered meshes

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



# Then, why collocated arrangements are so popular?

- STAR-CCM+



SIEMENS



- ANSYS-FLUENT



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- OpenFOAM

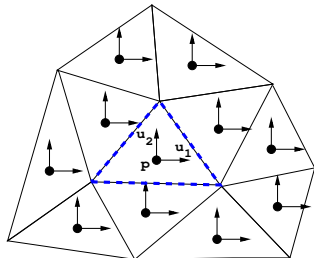
OpenFOAM®



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

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, ... **✓**



# Then, why collocated arrangements are so popular?

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

- STAR-CCM+



SIEMENS



- ANSYS-FLUENT



- Code-Saturne



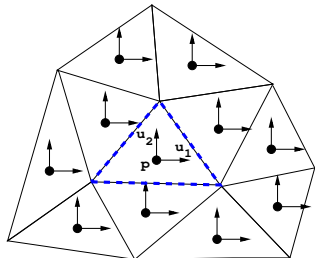
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# Pressure-velocity coupling on staggered grids

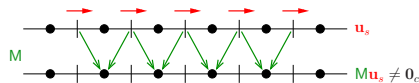
Works perfectly!



$u_s$

# Pressure-velocity coupling on staggered grids

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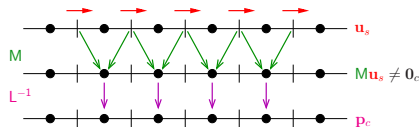


$Mu_s$



# Pressure-velocity coupling on staggered grids

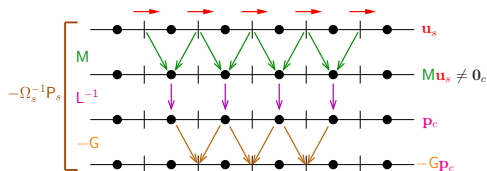
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$$\underbrace{L^{-1}Mu_s}_{p_c}$$

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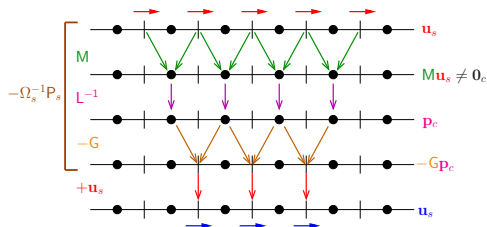
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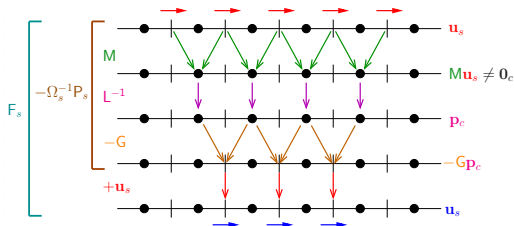
Works perfectly!



$$\mathbf{u}_s = \mathbf{u}_s - \underbrace{\mathbf{G} \mathbf{L}^{-1} \mathbf{M}}_{\mathbf{P}_c} \mathbf{u}_s$$

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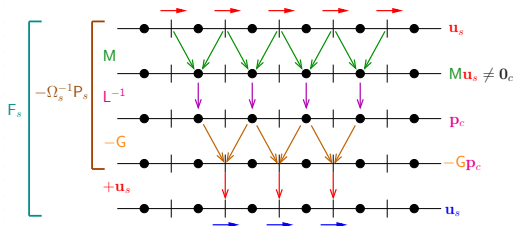
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$$\mathbf{u}_s = \mathbf{u}_s - \underbrace{\mathbf{G} \mathbf{L}^{-1} \mathbf{M}}_{\mathbf{P}_c} \mathbf{u}_s = (\mathbf{I} - \mathbf{\Omega}_s^{-1} \mathbf{P}_s) \mathbf{u}_s = \mathbf{F}_s \mathbf{u}_s$$

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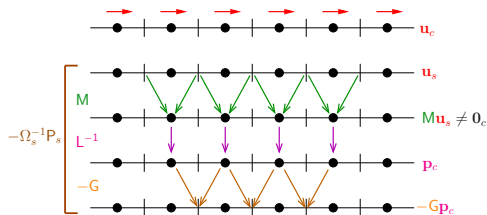


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# Pressure-velocity coupling on collocated grids

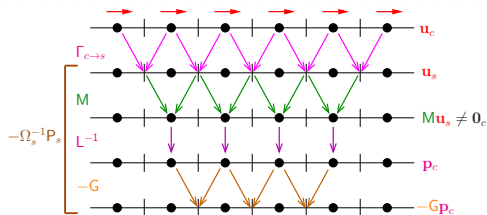
A vicious circle that cannot be broken...



$u_c$

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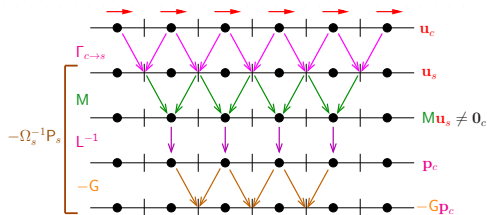
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$$\Gamma_{c \rightarrow s} u_c$$

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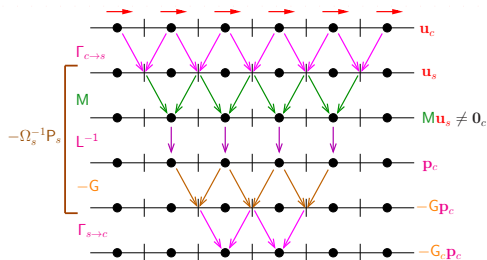


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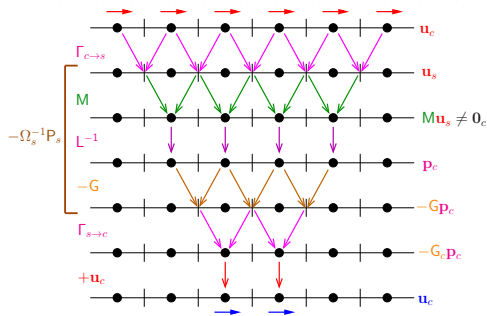
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$$- \Gamma_{s \rightarrow c} G L^{-1} M \Gamma_{c \rightarrow s} u_c$$

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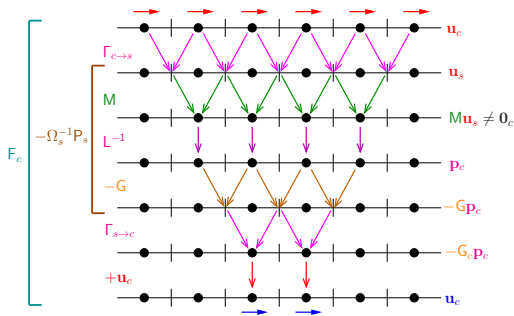
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$$u_c = u_c - \Gamma_{s \rightarrow c} G L^{-1} M \Gamma_{c \rightarrow s} u_c$$

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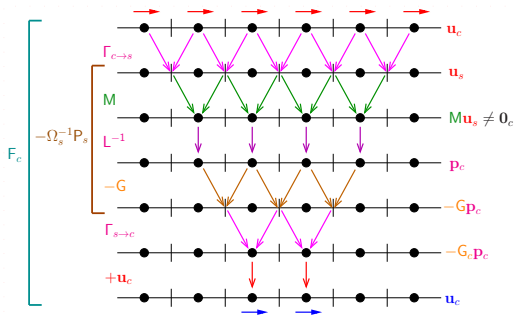
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$$u_c = u_c - \Gamma_{s \rightarrow c} G L^{-1} M \Gamma_{c \rightarrow s} u_c = F_c u_c$$

# Pressure-velocity coupling on collocated grids

A vicious circle that cannot be broken...



$$\mathbf{u}_c = \mathbf{u}_c - \Gamma_{s \rightarrow c} \mathbf{G} \mathbf{L}^{-1} \mathbf{M} \Gamma_{c \rightarrow s} \mathbf{u}_c = \mathbf{F}_c \mathbf{u}_c$$

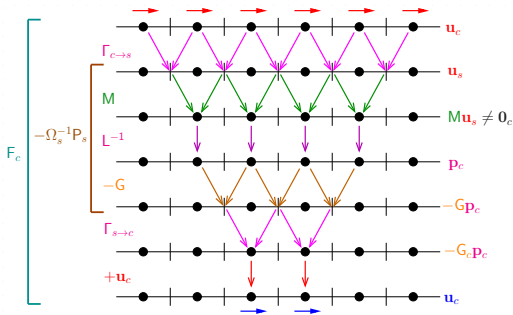
To preserve symmetry we impose  $\Gamma_{s \rightarrow c} = \Omega_c^{-1} \Gamma_{c \rightarrow s}^T \Omega_s$ . This leads to

$$\mathbf{M} \Gamma_{c \rightarrow s} \mathbf{u}_c = \mathbf{M} \Gamma_{c \rightarrow s} \mathbf{u}_c - \mathbf{L}_c \mathbf{L}^{-1} \mathbf{M} \Gamma_{c \rightarrow s} \mathbf{u}_c \approx \mathbf{0}_c \quad \times$$

where  $\mathbf{L}_c = -\mathbf{M} \Gamma_{c \rightarrow s} \Omega_c^{-1} \Gamma_{c \rightarrow s}^T \mathbf{M}$  (wide-stencil discrete Laplacian).

# Pressure-velocity coupling on collocated grids

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Moreover, **contribution to kinetic energy:**  $\mathbf{p}_c (\mathbf{L} - \mathbf{L}_c) \mathbf{p}_c \neq 0 \quad \times$

# 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:  $\mathbf{p}_c (L - L_c) \mathbf{p}_c \neq 0 \quad \mathbf{X}$

---

<sup>8</sup>F.X.Trias, O.Lehmkuhl, A.Oliva, C.D.Pérez-Segarra, R.W.C.P.Verstappen.  
*Symmetry-preserving discretization of Navier-Stokes equations on collocated unstructured grids*, **Journal of Computational Physics**, 258 (1): 246-267, 2014.

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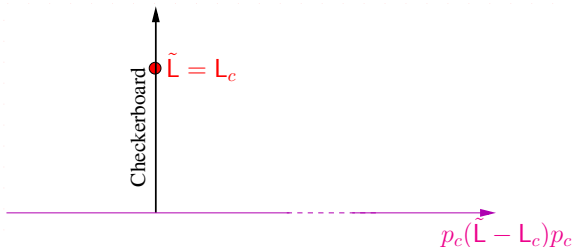
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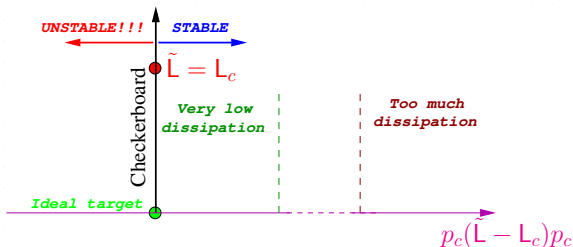


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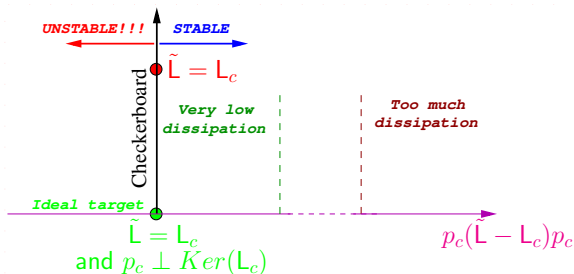
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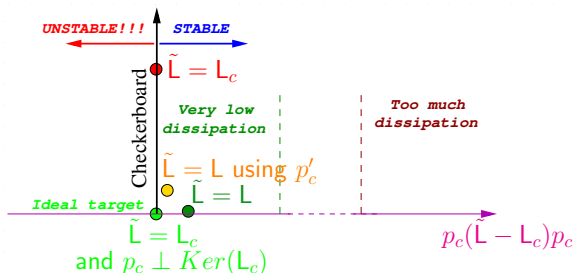
<sup>8</sup>Shashank, J.Larsson, G.laccarino. A co-located incompressible Navier-Stokes solver with exact mass, momentum and kinetic energy conservation in the inviscid limit, *Journal of Computational Physics*, 229: 4425-4430,2010.

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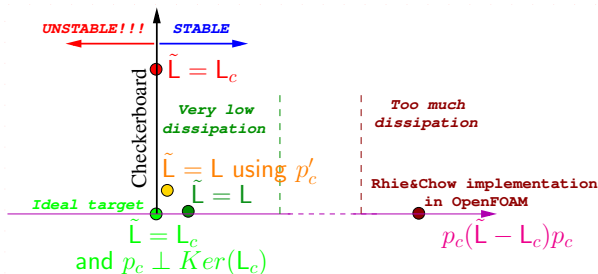
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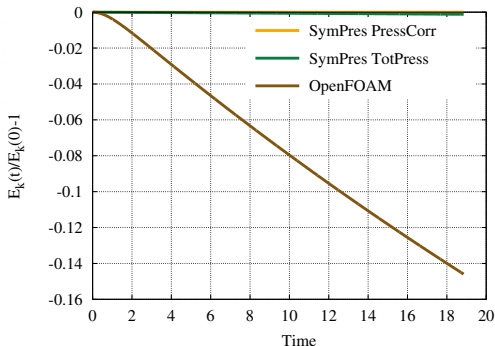
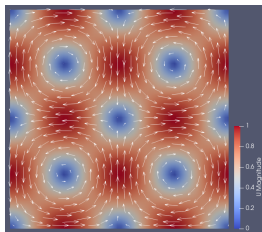
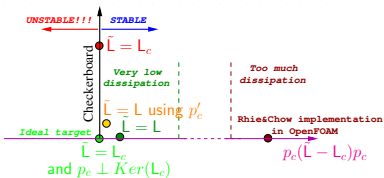
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# Pressure-velocity coupling on collocated grids

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

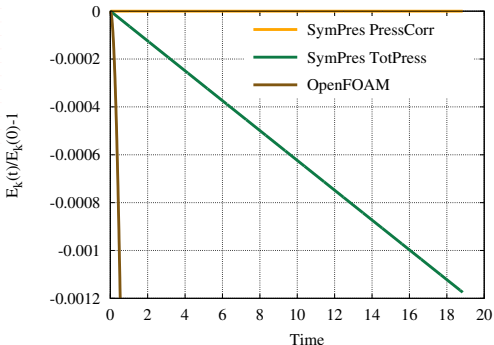
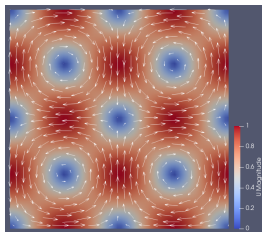
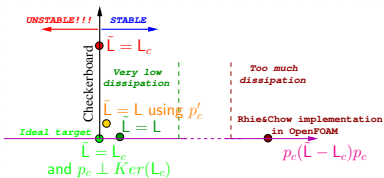


Results for an inviscid Taylor-Green vortex<sup>9</sup>

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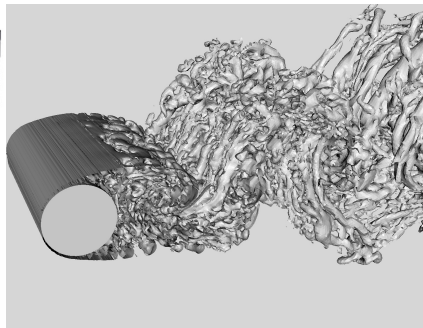
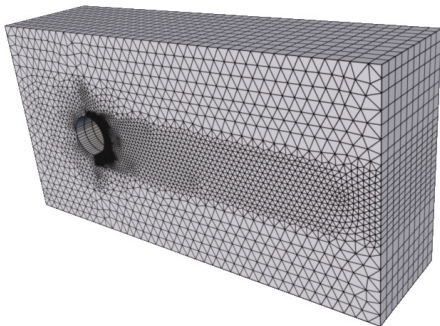
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# Pressure-velocity coupling on collocated grids

## Examples of simulations

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

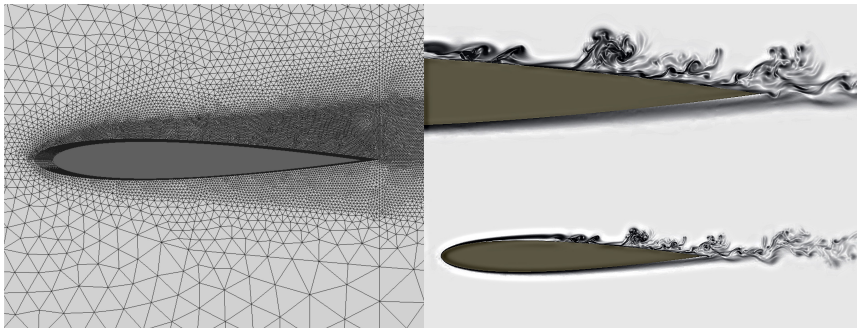


<sup>10</sup>R.Borrell, O.Lehmkuhl, F.X.Trias, A.Oliva. *Parallel Direct Poisson solver for discretizations with one Fourier diagonalizable direction*. **Journal of Computational Physics**, 230:4723-4741, 2011.

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## Examples of simulations

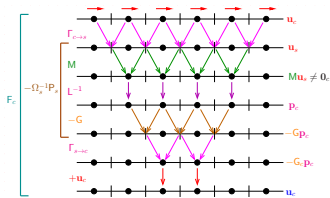
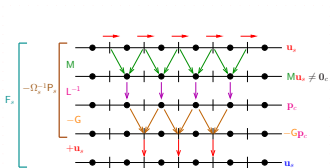
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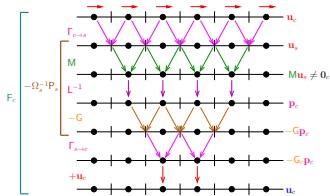
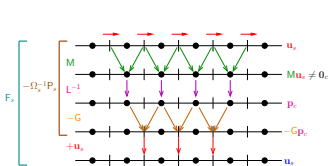


# Are staggered and collocated so different at the end?



$$\text{Collocated: } \mathbf{u}_c^{n+1} = \underbrace{(\mathbf{I}_c - \Gamma_{s \rightarrow c} \Omega_s^{-1} \mathbf{P}_s \Gamma_{c \rightarrow s})}_{\mathbf{F}_c} \underbrace{[\mathbf{I}_c + \partial_t^c]}_{\mathbf{T}_c} \mathbf{u}_c^n = \underbrace{\mathbf{F}_c \mathbf{T}_c}_{\mathbf{NS}_c} \mathbf{u}_c^n$$

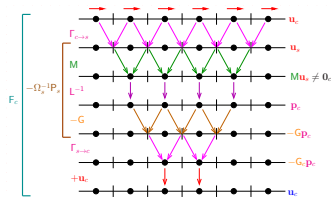
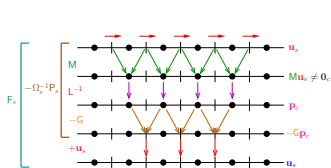
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$$\text{Naïve collocated: } \mathbf{u}_c^{n+1} = \underbrace{\Gamma_{s \rightarrow c} \mathbf{F}_s \Gamma_{c \rightarrow s} \mathbf{T}_c}_{\tilde{\mathbf{NS}}_c} \mathbf{u}_c^n$$

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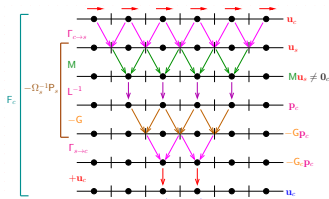
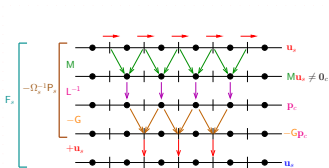


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$$\text{Naïve collocated: } \mathbf{u}_c^{n+1} = \underbrace{\Gamma_{s \rightarrow c} \mathbf{F}_s \Gamma_{c \rightarrow s} \mathbf{T}_c}_{\widetilde{\mathbf{NS}}_c} \mathbf{u}_c^n$$

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# Are staggered and collocated so different at the end?



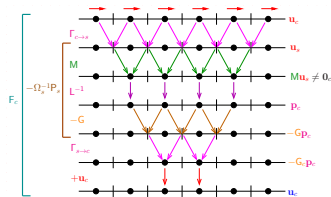
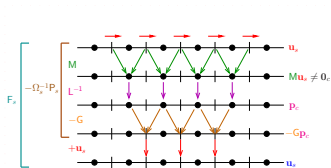
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$$\text{Naïve staggered: } \mathbf{u}_s^{n+1} = \underbrace{\mathbf{F}_s \Gamma_{c \rightarrow s} \mathbf{T}_c \Gamma_{s \rightarrow c}}_{\widetilde{\mathbf{N}}\mathbf{S}_s} \mathbf{u}_s^n$$

$$\Gamma_{s \rightarrow c} (\widetilde{\mathbf{N}}\mathbf{S}_s)^n = (\widetilde{\mathbf{N}}\mathbf{S}_c)^n \Gamma_{c \rightarrow s}$$

# Are staggered and collocated so different at the end?



$$\text{Collocated: } \mathbf{u}_c^{n+1} = \underbrace{(\mathbf{I}_c - \Gamma_{s \rightarrow c} \Omega_s^{-1} \mathbf{P}_s \Gamma_{c \rightarrow s})}_{\mathbf{F}_c} \underbrace{[\mathbf{I}_c + \partial_t^c]}_{\mathbf{T}_c} \mathbf{u}_c^n = \underbrace{\mathbf{F}_c \mathbf{T}_c}_{\mathbf{NS}_c} \mathbf{u}_c^n$$

$$\text{Staggered: } \mathbf{u}_s^{n+1} = \underbrace{(\mathbf{I}_s - \Omega_s^{-1} \mathbf{P}_s)}_{\mathbf{F}_s} \underbrace{[\mathbf{I}_s + \Gamma_{c \rightarrow s} \partial_t^c \Gamma_{s \rightarrow c}]}_{\mathbf{T}_s} \mathbf{u}_s^n$$

# Can we have a staggered formulation based only on collocated operators?

Then, it could be easily implemented in existing collocated codes such as OpenFOAM

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Similar approaches have been proposed in the literature before<sup>11,12,13,14,15</sup>.

<sup>11</sup> B.Perot. *Conservative properties of unstructured staggered meshes chemes*. **Journal of Comp. Physics**, 159: 58-89, 2000

<sup>12</sup> X.Zhang, D.Schmidt, B.Perot. *Accuracy and conservation properties of a three-dimensional unstructured staggered mesh scheme for fluid dynamics*. **Journal of Computational Physics**, 175: 764-791, 2002.

<sup>13</sup> K.Mahesh, G.Constantinescu, P.Moin. *A numerical method for large-eddy simulation in complex geometries*. **Journal of Computational Physics**, 197: 215-240, 2004.

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<sup>15</sup> L.Jofre, O.Lehmkuhl, J.Ventosa, F.X.Trias, A.Oliva. *Conservation properties of unstructured finite-volume mesh schemes for the Navier-Stokes equations*. **Numerical Heat Transfer, Part B**, 65:1-27, 2014.

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Similar approaches have been proposed in the literature before<sup>11,12,13,14,15</sup>.

**Research question:** then, why at the end collocated approach seems to be the winner?

- STAR-CCM+



- SIEMENS



- ANSYS-FLUENT



- Code-Saturne



- OpenFOAM



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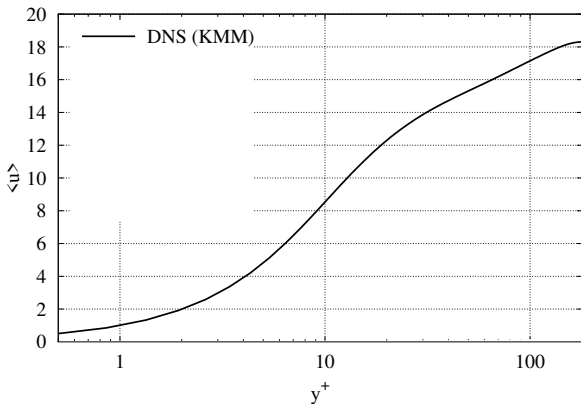
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# Results for a turbulent channel flow at $Re_\tau = 180$

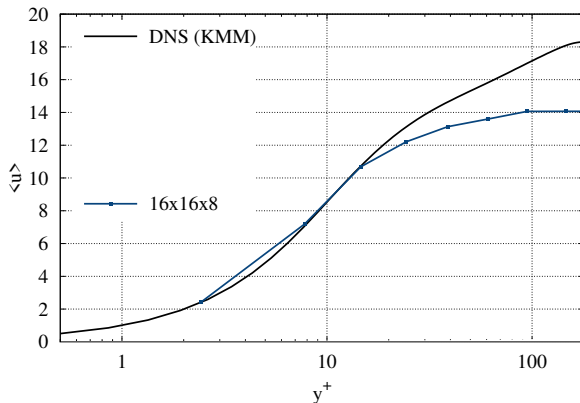
Staggered  $C_s^0$ : 
$$\mathbf{u}_s^{n+1} = \underbrace{(\mathbf{I}_s - \Omega_s^{-1} \mathbf{P}_s)}_{\mathbf{F}_s} \underbrace{[\mathbf{I}_s + \Gamma_{c \rightarrow s} \partial_t^c \Gamma_{s \rightarrow c}]}_{\mathbf{T}_s} \mathbf{u}_s^p$$





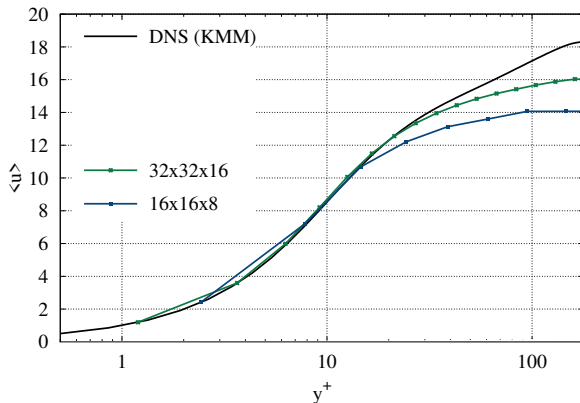
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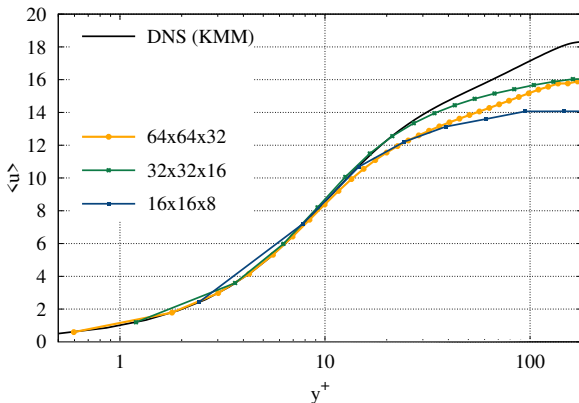
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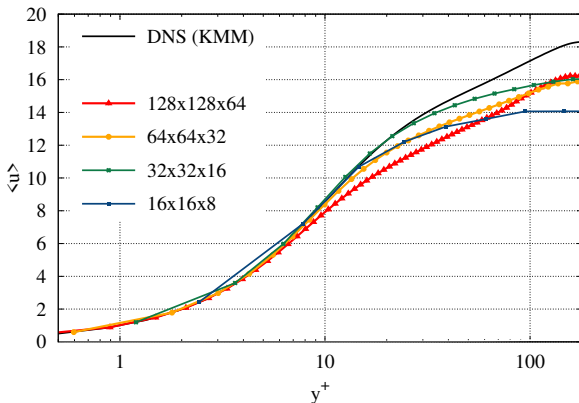
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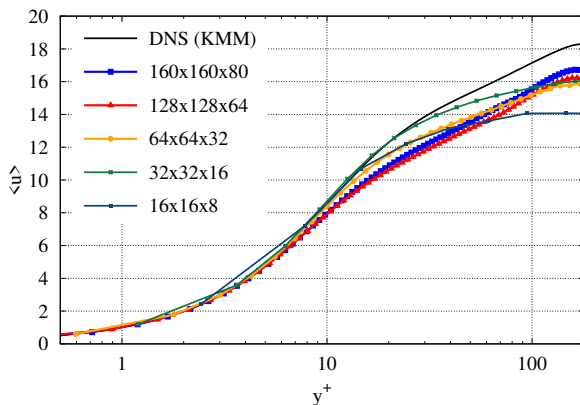
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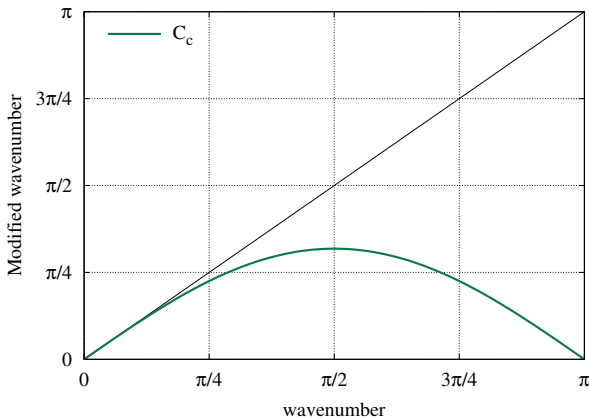
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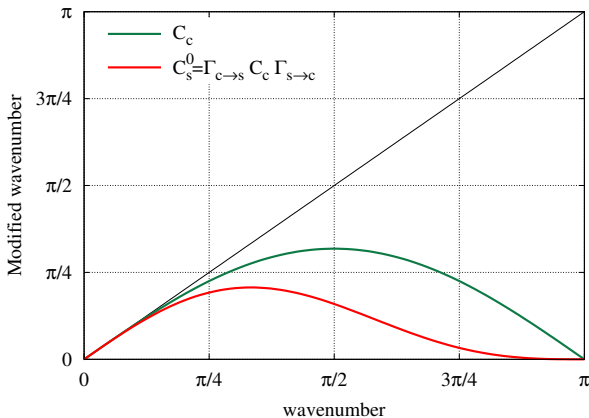
# Dispersion errors analysis

Staggered  $C_s^0$ : 
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# Dispersion errors analysis

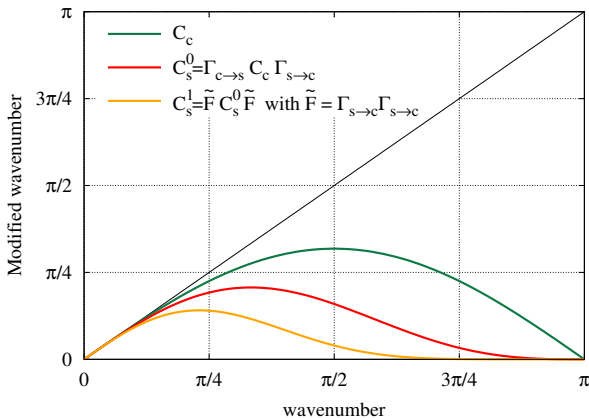
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# Dispersion errors analysis

$$\text{Staggered } C_s^1: \quad \mathbf{u}_s^{n+1} = \underbrace{(I_s - \Omega_s^{-1} P_s)}_{F_s} \underbrace{\left[ I_s + \overbrace{\tilde{F} \Gamma_{c \rightarrow s} \partial_t^c \Gamma_{s \rightarrow c} \tilde{F}}^{u_s^P} \right]}_{T_s} \mathbf{u}_s$$

Filter:  $\tilde{F} = \Gamma_{s \rightarrow c} \Gamma_{c \rightarrow s}$  ( $\tilde{F} = \tilde{F}^T$  and positive semi-definite)

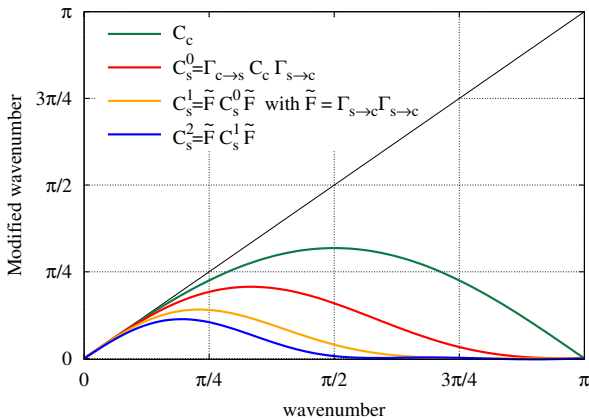




# Dispersion errors analysis

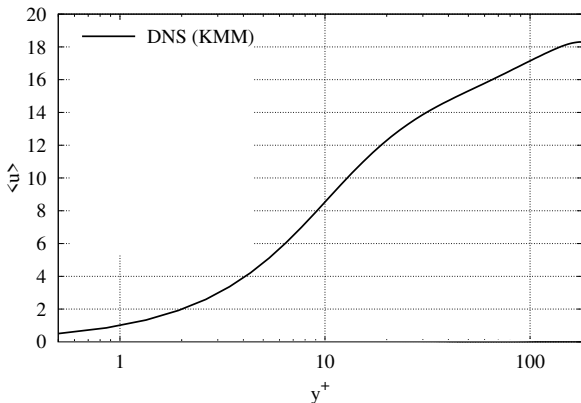
$$\text{Staggered } C_s^2: \quad \underbrace{\mathbf{u}_s^{n+1}}_{\mathbf{F}_s} = \underbrace{(\mathbf{I}_s - \Omega_s^{-1} \mathbf{P}_s)}_{\mathbf{F}_s} \underbrace{\left[ \mathbf{I}_s + \underbrace{\tilde{\mathbf{F}} \tilde{\mathbf{F}} \Gamma_{c \rightarrow s} \partial_t^c \Gamma_{s \rightarrow c} \tilde{\mathbf{F}} \tilde{\mathbf{F}}}_{\mathbf{T}_s} \right]}_{\mathbf{T}_s} \underbrace{\mathbf{u}_s^n}_{\mathbf{u}_s^P}$$

Filter:  $\tilde{\mathbf{F}} = \Gamma_{s \rightarrow c} \Gamma_{c \rightarrow s}$  ( $\tilde{\mathbf{F}} = \tilde{\mathbf{F}}^T$  and positive semi-definite)



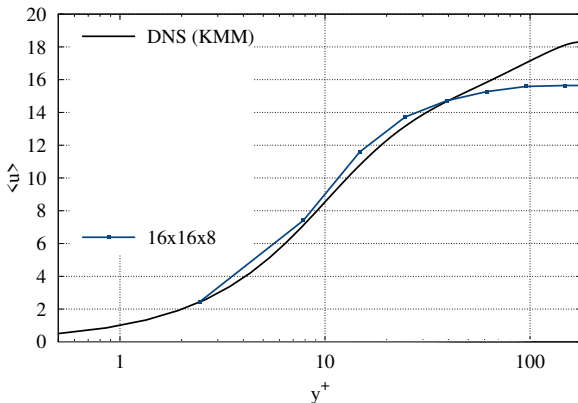
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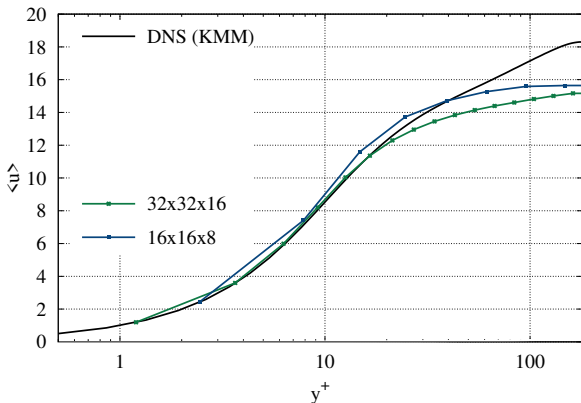
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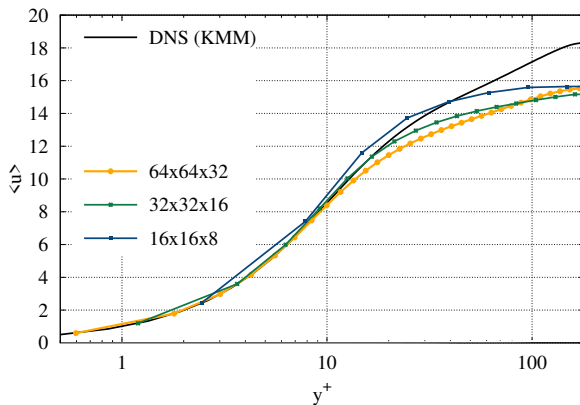
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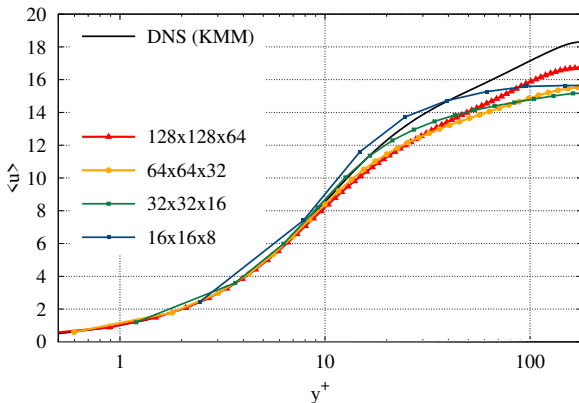
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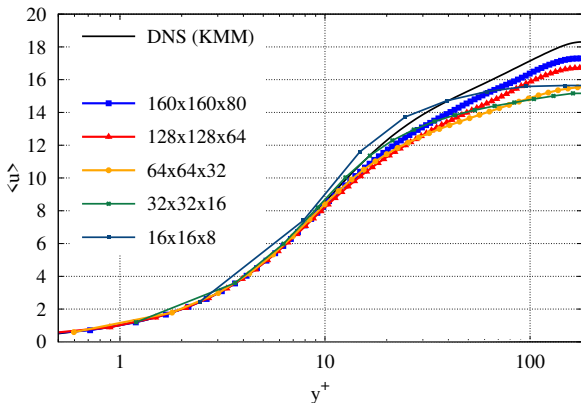
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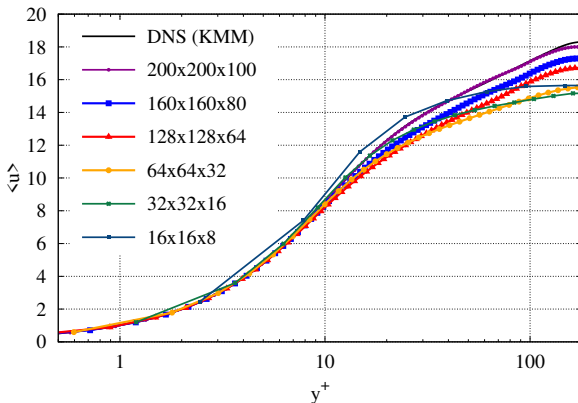
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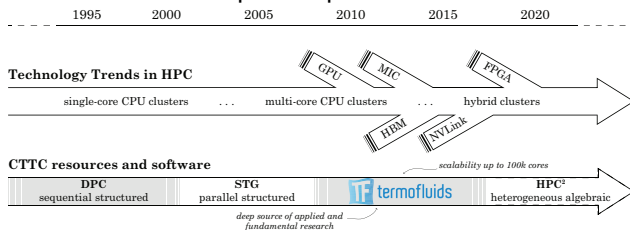




# Algebra-based approach naturally leads to portability

## Research question #2:

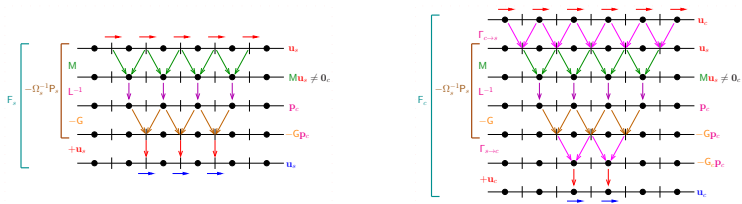
- How can we develop **portable** and **efficient** CFD codes for large-scale simulations on modern supercomputers?



**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. NUMA-aware execution strategies for CFD are presented in this conference<sup>16</sup>.

<sup>16</sup>X.Álvarez, A.Gorobets, F.X.Trias, A.Oliva. *NUMA-aware strategies for the efficient execution of CFD simulations on CPU supercomputers* ParCFD2021. Don't miss it!

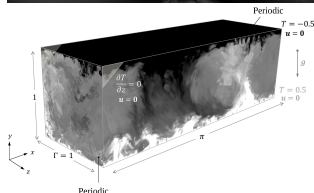
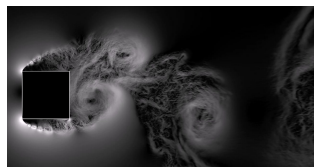
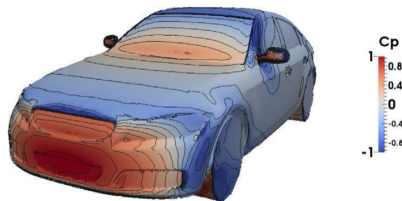
# Algebra-based approach naturally leads to portability, to simple and analyzable formulations



$$\text{Collocated: } \mathbf{u}_c^{n+1} = \underbrace{(\mathbf{I}_c - \Gamma_{s \rightarrow c} \Omega_s^{-1} \mathbf{P}_s \Gamma_{c \rightarrow s})}_{\mathbf{F}_c} \underbrace{[\mathbf{I}_c + \partial_t^c]}_{\mathbf{T}_c} \mathbf{u}_c^n = \underbrace{\mathbf{F}_c \mathbf{T}_c}_{\mathbf{NS}_c} \mathbf{u}_c^n$$

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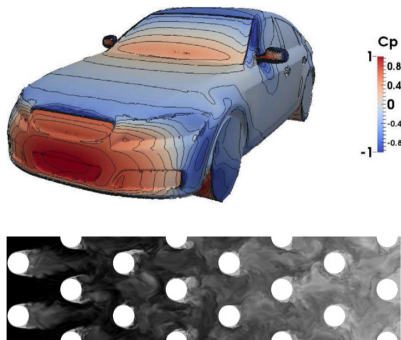
Algebra-based approach naturally leads to portability, to simple and analyzable formulations and opens the door to new strategies<sup>17</sup> to improve its performance...



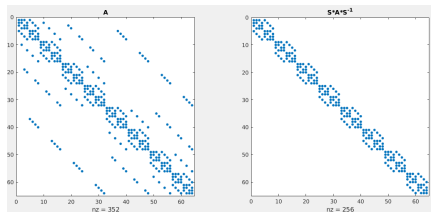
<sup>17</sup>

A. Alsalti, X. Álvarez, F.X. Trias, A. Gorobets, A. Oliva. *A highly portable heterogeneous implementation of a Poisson solver for flows with one periodic direction* ParCFD2021. Don't miss it!

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

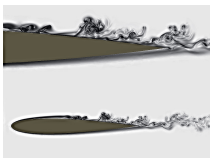


SpMMV can be used  $\implies$  **higher AI**

<sup>17</sup> A. Alsalti, X. Álvarez, F.X. Trias, A. Gorobets, A. Oliva. *A highly portable heterogeneous implementation of a Poisson solver for flows with one periodic direction* ParCFD2021. Don't miss it!

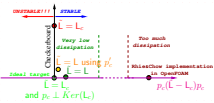
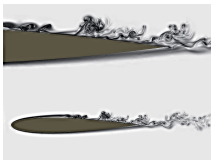
## Concluding remarks

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



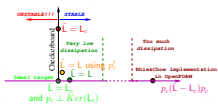
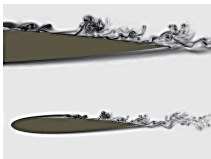
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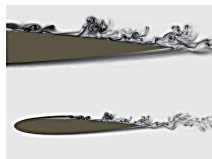
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- Despite this, the CFD community have generally adopted collocated formulations due to the inherent **difficulties** to formulate a simple and robust **staggered discretization of momentum**.  
 ⇒ A potential solution has been presented here...



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- Code-Saturne
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- EDF
-

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- SIEMENS 
- EDF 
- GPL 

On-going research:

- Complete the analysis for higher  $Re_\tau$
- Test for complex geometries using unstructured meshes



Thank you for your virtual  
attendance